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(54) METAL COORDINATION COMPOUND, LUMINESCENCE DEVICE AND DISPLAY APPARATUS

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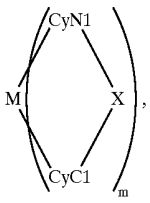
(57) **ABSTRACT**

An organic EL device includes a luminescence layer containing, as a luminescent material allowing a high-luminescence and high-efficiency luminescence for a long period of time, a metal coordination compound represented by the following formula (1): LmML'n, wherein M denotes Ir, Pt, Ph or Pd; L denotes a bidentate ligand; L' denotes a bidentate ligand different from L; m is an integer of 1, 2 or 3; and n is an integer of 0, 1 or 2 with the proviso that the sum of m and n is 2 or 3. The partial structure MLm is represented by a formula (2) or a formula (3) shown below, and the partial structure ML'n is represented by a formula (4) or a formula (5) shown below:

(2)



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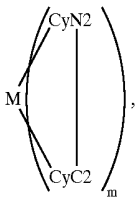

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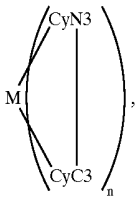

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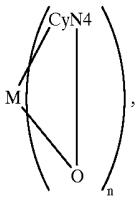


wherein CyN1, CyN2 and CyN3 independently denote a substituted or unsubstituted cyclic group containing a nitrogen atom connected to M; CyN4 denotes a cyclic group containing 8-quinoline or its derivative having a nitrogen atom connected to M; CyC1, CyC2 and CyC3 independently denote a substituted or unsubstituted cyclic group containing a carbon atom connected to M, with the proviso that the metal coordination compound is represented by the formula (2) when n is 0.

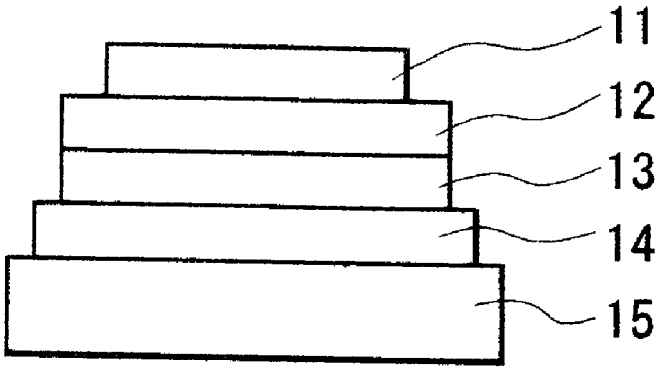


FIG. 1A

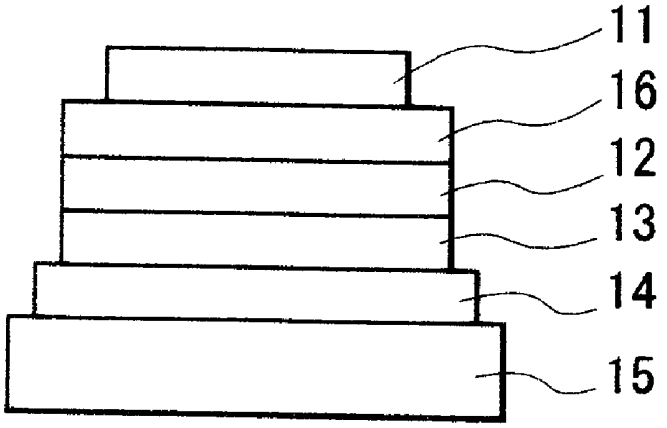


FIG. 1B

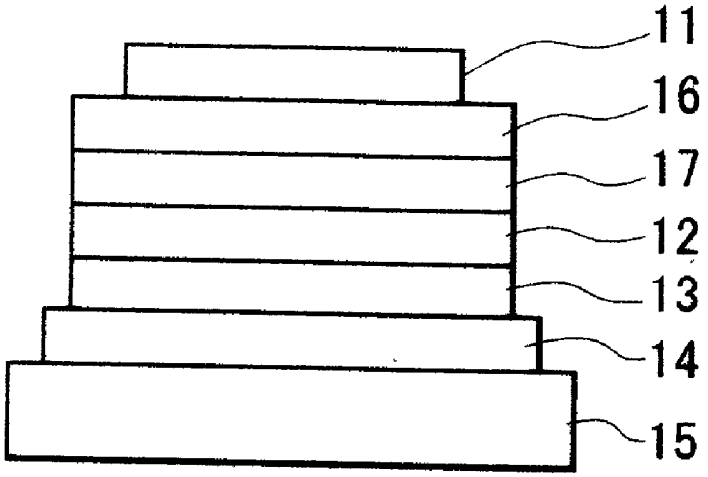


FIG. 1C

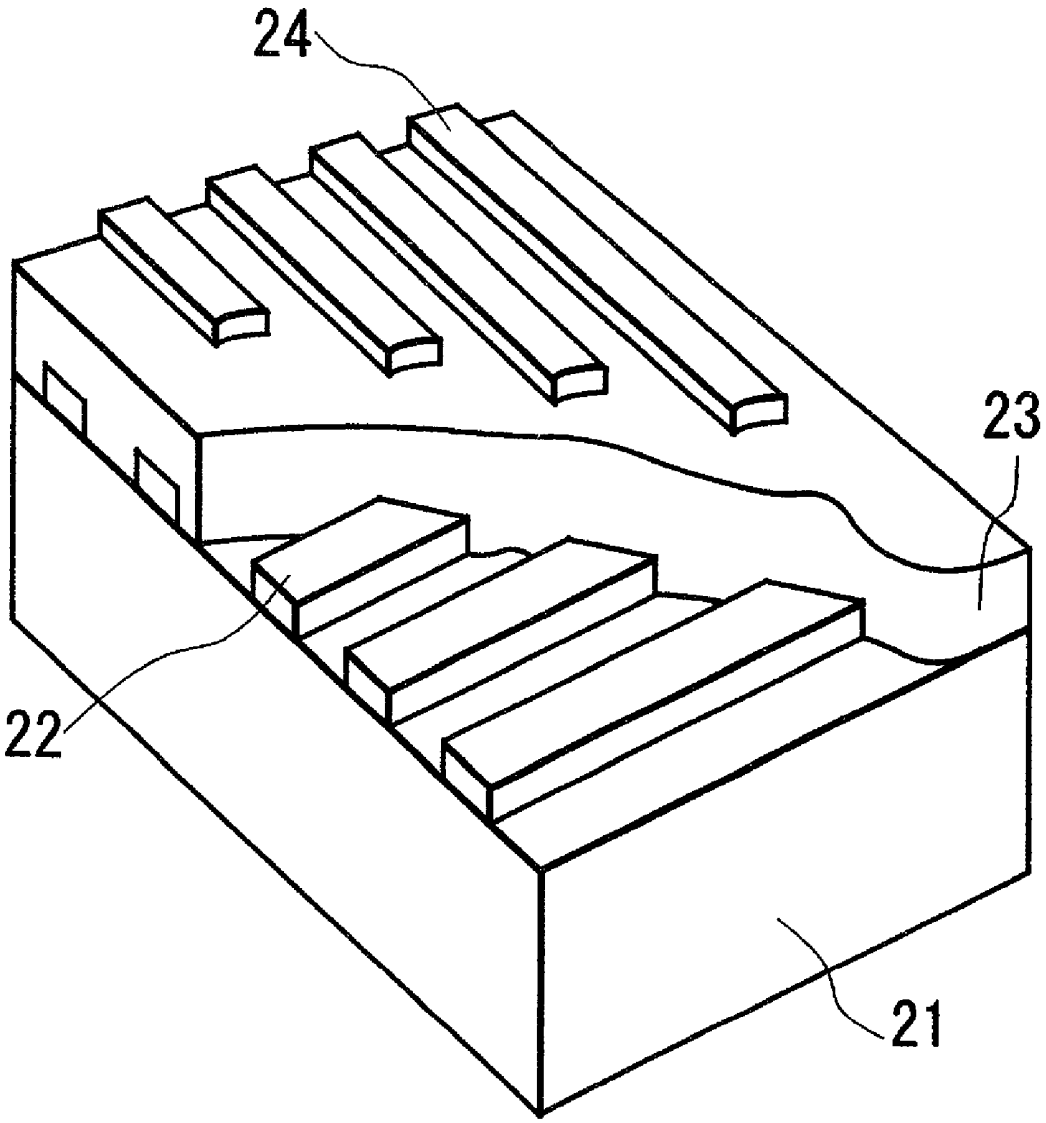


FIG. 2

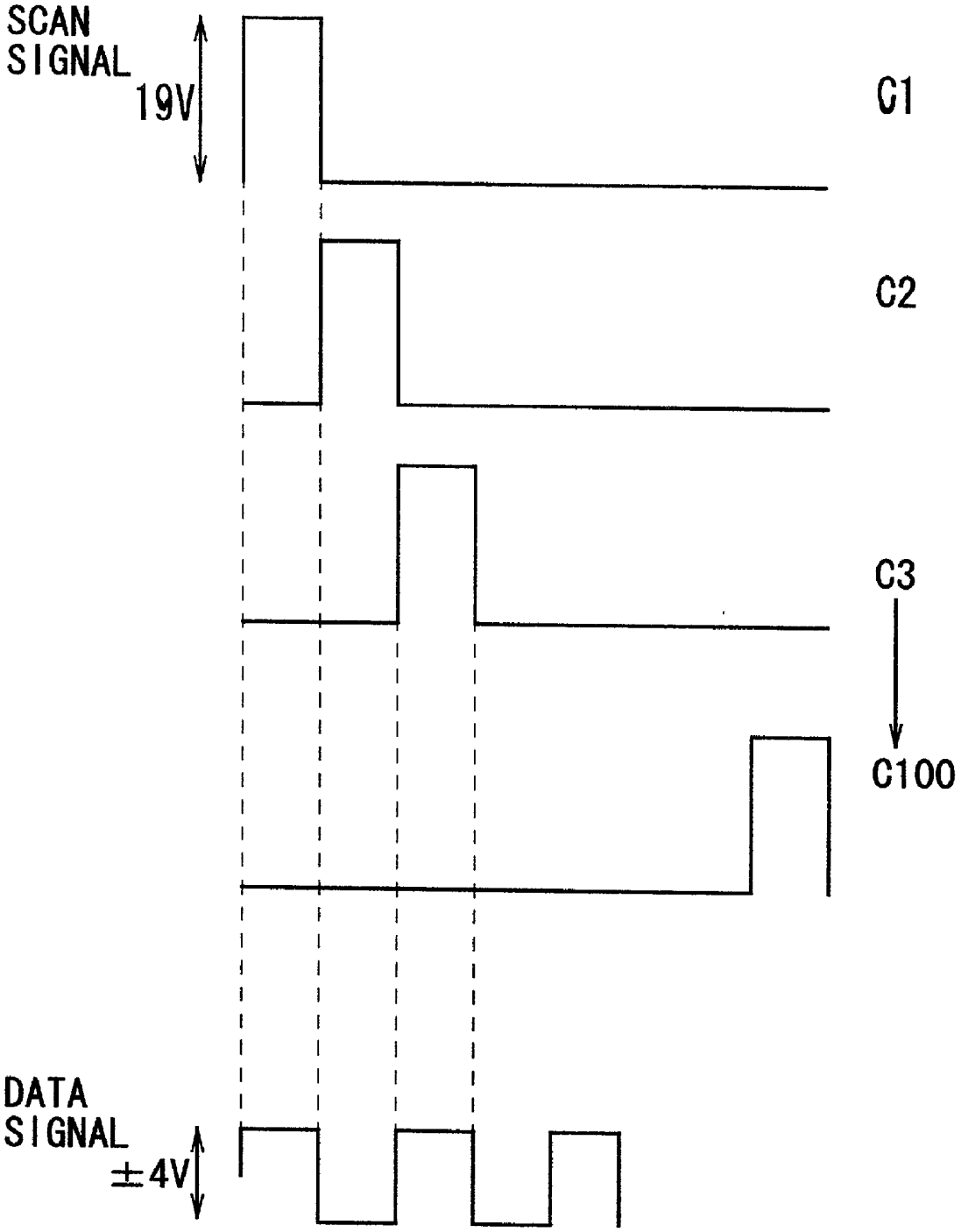


FIG. 3

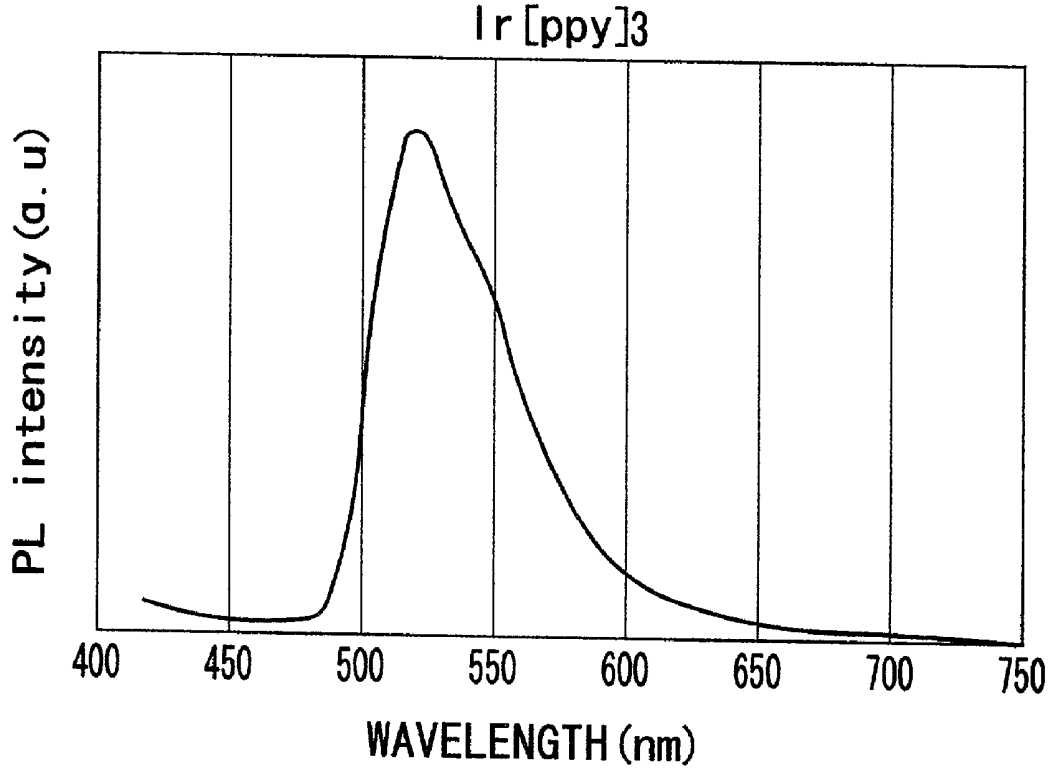
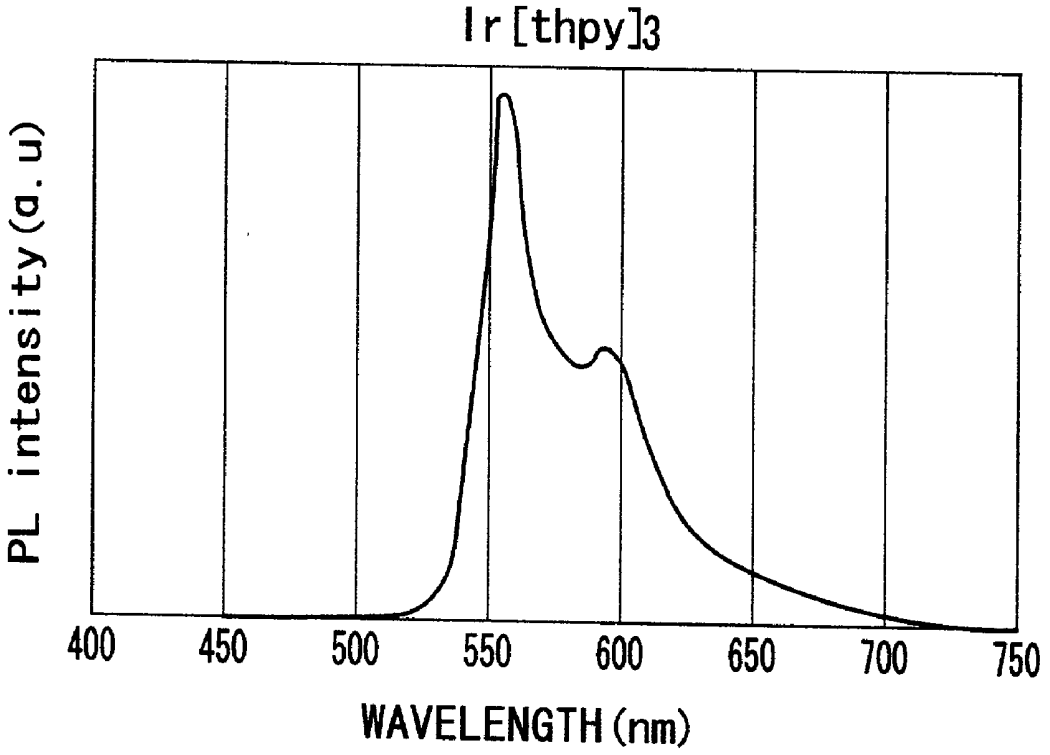

Ir[ppy]3
PL intensity(a.u)
400
450
500
550
600
650
700
750
WAVELENGTH (nm)

FIG. 4A


Ir[thpy]3
PL intensity(a.u)
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450
500
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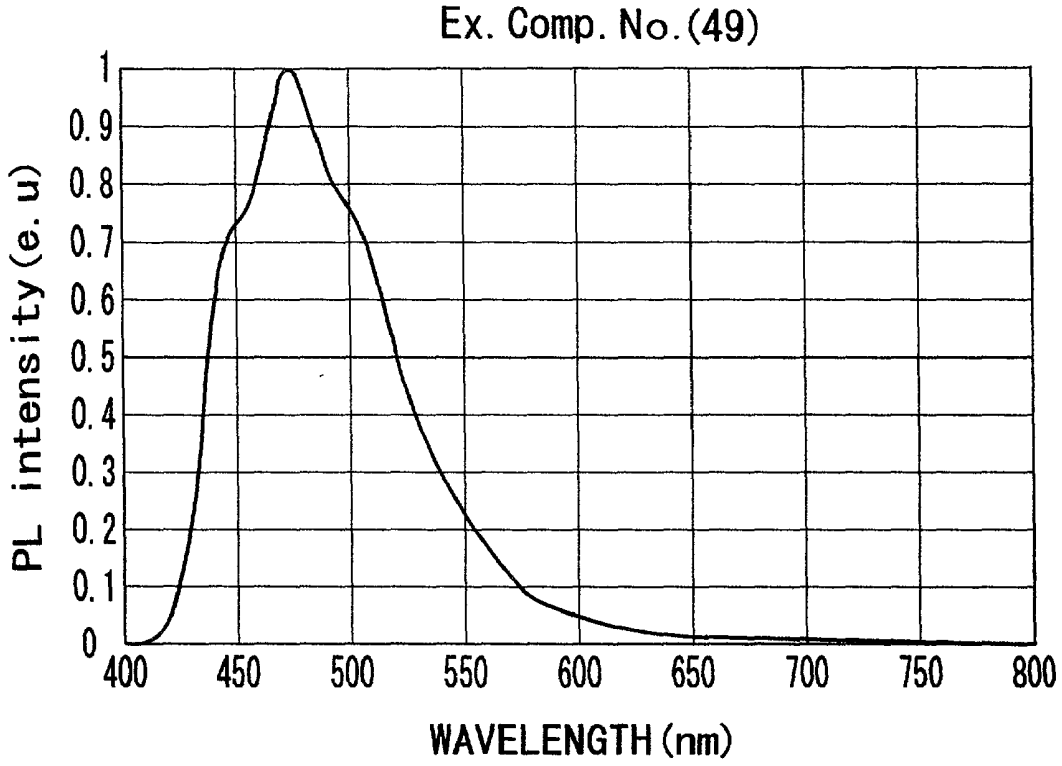
600
650
700
750
WAVELENGTH (nm)

FIG. 4B


Ex. Comp. No.(49)
PL intensity (e.u)
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0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
400
450
500
550
600
650
700
750
800
WAVELENGTH (nm)

FIG. 5

METAL COORDINATION COMPOUND, LUMINESCENCE DEVICE AND DISPLAY APPARATUS

FIELD OF THE INVENTION AND RELATED ART

[0001] The present invention relates to a metal coordination compound, an organic luminescence device using the metal coordination compound and a display apparatus using the device. More specifically, the present invention relates to an organic metal coordination compound having a formula (1) appearing hereinafter as a luminescence material so as to allow stable luminescence efficiency, an organic luminescence device using the metal coordination compound and a display apparatus including the luminescence device.

[0002] An organic electroluminescence (EL) device has been extensively studied as a luminescence device with a high responsiveness and high efficiency.

[0003] The organic EL device generally has a sectional structure as shown in **FIG. 1A** or 1B (e.g., as described in "Macromol. Symp.", 125, pp. 1-48 (1997)).

[0004] Referring to the figures, the EL device generally has a structure including a transparent substrate **15**, a transparent electrode **14** disposed on the transparent substrate **15**, a metal electrode **11** disposed opposite to the transparent electrode **14**, and a plurality of organic (compound) layers, as luminescence function layers, disposed between the transparent electrode **14** and the metal electrode **11**.

[0005] Referring to **FIG. 1A**, the EL device in this embodiment has two organic layers including a luminescence layer **12** and a hole transport layer **13**.

[0006] The transparent electrode **14** may be formed of a film of ITO (indium tin oxide) having a larger work function to ensure a good hole injection performance into the hole transport layer. On the other hand, the metal electrode **11** may be formed of a layer of aluminum, magnesium, alloys thereof, etc., having a smaller work function to ensure a good electron injection performance into the organic layer(s).

[0007] These (transparent and metal) electrodes **14** and **11** may be formed in a thickness of 50-200 nm.

[0008] The luminescence layer **12** may be formed of, e.g., aluminum quinolinol complex (representative example thereof may include Alq3 described hereinafter) having an electron transporting characteristic and a luminescent characteristic. The hole transport layer **13** may be formed of, e.g., biphenyldiamine derivative (representative example thereof may include α-NPD described hereinafter) having an electron donating characteristic.

[0009] The above-described EL device exhibits a rectification characteristic, so that when an electric field is applied between the metal electrode **11** as a cathode and the transparent electrode **14** as an anode, electrons are injected from the metal electrode **11** into the luminescence layer **12** and holes are injected from the transparent electrodes **14**.

[0010] The thus-injected holes and electrons are recombined within the luminescence layer **12** to produce excitons placed in an excited state, thus causing luminescence at the time of transition of the excitons to a ground state. At that time, the hole transport layer **13** functions as an electron-blocking layer to increase a recombination efficiency at the boundary between the luminescence layer **12** and the hole transport layer **13**, thus enhancing a luminescence efficiency.

[0011] Referring to **FIG. 1B**, in addition to the layers shown in **FIG. 1A**, an electron transport layer **16** is disposed between the metal electrode **11** and the luminescence layer **12**, whereby an effective carrier blocking performance can be ensured by separating functions of luminescence, electron transport and hole transport, thus allowing effective luminescence.

[0012] The electron transport layer **16** may be formed of, e.g., oxadiazole derivatives.

[0013] In ordinary organic EL devices, fluorescence caused during a transition of luminescent center molecule from a singlet excited state to a ground state is used as luminescence.

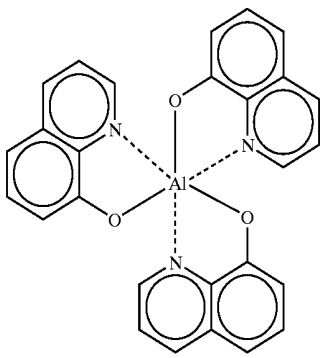
[0014] On the other hand, different from the above fluorescence (luminescence) via singlet exciton, phosphorescence (luminescence) via triplet exciton has been studied for use in organic EL device as described in, e.g., "Improved energy transfer in electrophosphorescent device" (D. F. O'Brien et al., Applied Physics Letters, Vol. 74, No. 3, pp. 442-444 (1999)) and "Very high-efficiency green organic light-emitting devices based on electrophosphorescence" (M. A. Baldo et al., Applied Physics Letters, Vol. 75, No. 1, pp. 4-6 (1999)).

[0015] The EL devices shown in these documents may generally have a sectional structure shown in **Figure 1C**.

[0016] Referring to **FIG. 1C**, four organic layers including a hole transfer layer **13**, a luminescence layer **12**, an exciton diffusion-prevention layer **17**, and an electron transport layer **16** are successively formed in this order on the transparent electrode (anode) **14**.

[0017] In the above documents, higher efficiencies have been achieved by using four organic layers including a hole transport layer **13** of α-NPD (shown below), an electron transport layer **16** of Alq3 (shown below), an exciton diffusion-prevention layer **17** of BPC (shown below), and a luminescence layer **12** of a mixture of CPB (shown below) as a host material with $Ir(ppy)_3$ (shown below) or PtOEP (shown below) as a guest phosphorescence material doped into CBP at a concentration of ca. 6 wt. %.

Alq3



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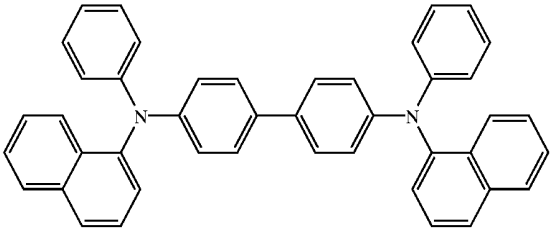
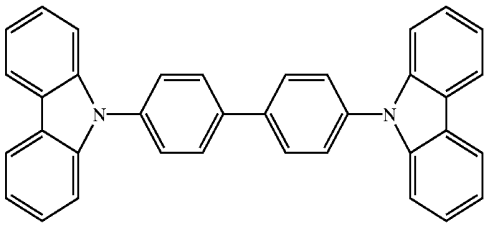
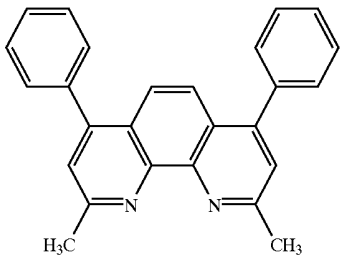
α-NPD



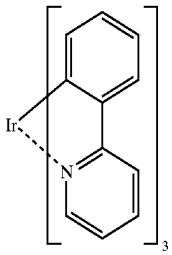
CBP

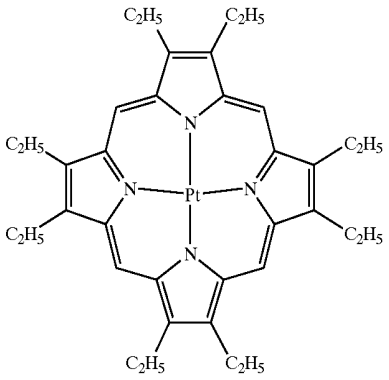


BCP



Ir(ppy)3





[0018] Alq3: tris(8-hydroxyquinoline) aluminum (aluminum-quinolinol complex),

[0019] α-NPD: N4,N4'-di-naphthalene-1-yl-N4,N4'-diphenyl-biphenyl-4,4'-diamine (4,4'-bis[N-(1-naphthyl)-N-phenyl-amino]biphenyl),

[0020] CBP: 4,4'-N,N'-dicarbazole-biphenyl,

[0021] BCP: 2,9-dimethyl-4,7-diphenyl-1,10-phenan-throline,

[0022] $Ir(ppy)_3$: fac tris(2-phenylpyridine)iridium (iridium-phenylpyridine complex), and

[0023] PtOE: 2,3,7,8,12,13,17,18-octaethyl-21H, 23H-porphine platinum (platinum-octaethyl porphine complex).

[0024] The phosphorescence (luminescence) material used in the luminescence layer **12** has particularly attracted notice. This is because the phosphorescence material is expected to provide a higher luminescence efficiency in principle.

[0025] More specifically, in the case of the phosphorescence material, excitons produced by recombination of carriers comprise singlet excitons and triplet excitons presented in a ratio of 1:3. For this reason, when fluorescence caused during the transition from the singlet excited state to the ground state is utilized, a resultant luminescence efficiency is 25% (as upper limit) based on all the produced excitons in principle.

[0026] On the other hand, in the case of utilizing phosphorescence caused during transition from the triplet excited state, a resultant luminescence efficiency is expected to be at least three times that of the case of fluorescence in principle. In addition thereto, if intersystem crossing from the singlet excited state (higher energy level) to the triplet excited state is taken into consideration, the luminescence efficiency of phosphorescence can be expected to be 100% (four times that of fluorescence) in principle.

[0027] The use of phosphorescence based on transition from the triplet excited state has also been proposed in, e.g., Japanese Laid-Open Patent Application (JP-A) 11-329739, JP-A 11-256148 and JP-A 8-319482.

[0028] However, the above-mentioned organic EL devices utilizing phosphorescence have accompanied with problems of a lower luminescence efficiency and stability thereof (luminescent deterioration) particularly in an energized state.

[0029] The reason for luminescent deterioration has not been clarified as yet but may be attributable to such a phenomenon that the life of triplet exciton is generally longer than that of singlet exciton by at least three digits, so that molecule is placed in a higher-energy state for a long period to cause reaction with ambient substance, formation of exciplex or excimer, change in minute molecular structure, structural change of ambient substance, etc.

[0030] Accordingly, a phosphorescence material for the (electro)phosphorescence EL device is required to provide a higher luminescence efficiency and a higher stability, to the EL device.

SUMMARY OF THE INVENTION

[0031] An object of the present invention is to provide a metal coordination compound as a material suitable for an organic layer of a luminescence device capable of providing a high-efficiency luminescent state at a high brightness (or luminance) for a long period while maintaining stability of the device.

[0032] Another object of the present invention is to provide a metal coordination compound allowing a higher phosphorescence yield and controlled emission (luminescence) wavelength as a phosphorescence (luminescence) material.

[0033] A further object to the present invention is to provide a metal coordination compound, as a multi-functional luminescence material, having not only a controlled luminescent characteristic but also controlled electrical characteristic, in view of a significance of the electrical characteristic of a luminescence material alone in the case where the luminescence material is employed in an organic EL device and is supplied with a current for luminescence.

[0034] A still further object of the present invention is to provide an organic luminescence device using the metal coordination compound and a display apparatus including the organic luminescence device.

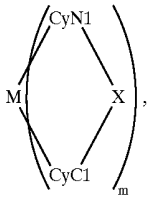
[0035] According to the present invention, there is provided a metal coordination compound represented by the following formula (1):

LmML'n (1),

[0036] wherein M denotes Ir, Pt, Ph or Pd; L denotes a bidentate ligand; L' denotes a bidentate ligand different from L; m is an integer of 1, 2 or 3; and n is an integer of 0, 1 or 2 with the proviso that the sum of m and n is 2 or 3,

[0037] the partial structure MLm being represented by a formula (2) or a formula (3) shown below, and the partial structure ML'n being represented by a formula (4) or a formula (5) shown below:

(2)



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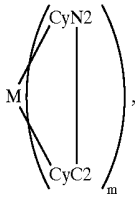

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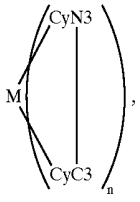

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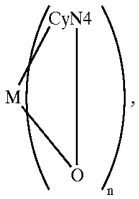
(5)



[0038] wherein CyN1, CyN2 and CyN3 independently denote a substituted or unsubstituted cyclic group containing a nitrogen atom connected to M; CyN4 denotes a cyclic group containing 8-quinoline or its derivative having a nitrogen atom connected to M; CyC1, CyC2 and CyC3 independently denote a substituted or unsubstituted cyclic group containing a carbon atom connected to M,

[0039] each of substituents for CyN1, CyN2, CyN3, CyC1, CyC2 and CyC3 being selected from the group consisting of a halogen atom; cyano group; nitro group; a trialkylsilyl group containing three linear or branched alkyl groups each independently having 1-8 carbon atoms; a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom; and an aromatic ring group capable of having a substituent selected from the group consisting of a halogen atom; cyano group; nitro group; and a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C—C— and capable of including a hydrogen atom which can be replaced with a fluorine atom,

[0040] CyN1 and CyC1 being connected via a covalent group containing X which is represented by —O—, —S—, —CO—, —C(R1)(R2)— or —NR— where R1, R2 and R independently denote a hydrogen atom, a halogen atom, an alkyl group, an alkyl group substituted with a halogen atom, a phenyl group or a naphthyl group, and

[0041] CyN2 and CyC2, and CyN3 and CyC3 being independently connected via a covalent bond,

[0042] with the proviso that the metal coordination compound is represented by the formula (2) when n is 0.

[0043] The metal coordination compound of the present invention exhibits phosphorescence at the time of energy transfer from an excited state to a ground state to provide a high luminescence efficiency.

[0044] According to the present invention, there is also provided an organic luminescence device, comprising: a substrate, a pair of electrodes disposed on the substrate, and

a luminescence function layer disposed between the pair of electrodes comprising at least one species of an organic compound,

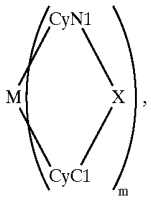
[0045] wherein the organic compound comprises a metal coordination compound represented by the following formula (1):

$$LmML'n \quad (1),$$

[0046] wherein M denotes Ir, Pt, Ph or Pd; L denotes a bidentate ligand; L' denotes a bidentate ligand different from L; m is an integer of 1, 2 or 3; and n is an integer of 0, 1 or 2 with the proviso that the sum of m and n is 2 or 3,

[0047] the partial structure MLm being represented by a formula (2) or a formula (3) shown below, and the partial structure ML'n being represented by a formula (4) or a formula (5) shown below:

(2)



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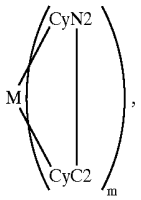

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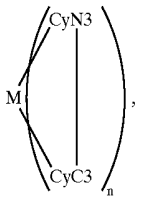

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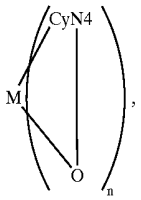


[0048] wherein CyN1, CyN2 and CyN3 independently denote a substituted or unsubstituted cyclic group containing a nitrogen atom connected to M; CyN4 denotes a cyclic group containing 8-quinoline or its derivative having a nitrogen atom connected to M; CyC1, CyC2 and CyC3 independently denote a substituted or unsubstituted cyclic group containing a carbon atom connected to M,

[0049] each of substituents for CyN1, CyN2, CyN3, CyC1, CyC2 and CyC3 being selected from the group consisting of a halogen atom; cyano group; nitro group; a trialkylsilyl group containing three linear or branched alkyl groups each independently having 1-8 carbon atoms; a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom; and an aromatic ring group capable of having a substituent selected from the group consisting of a halogen atom; cyano group; nitro group; and a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C—C— and capable of including a hydrogen atom which can be replaced with a fluorine atom,

[0050] CyN1 and CyC1 being connected via a covalent group containing X which is represented by —O—, —S—, —CO—, —C(R1)(R2)— or —NR— where R1, R2 and R independently denote a hydrogen atom, a halogen atom, an alkyl group, an alkyl group substituted with a halogen atom, a phenyl group or a naphthyl group, and

[0051] CyN2 and CyC2, and CyN3 and CyC3 being independently connected via a covalent bond,

[0052] with the proviso that the metal coordination compound is represented by the formula (2) when n is 0.

[0053] By applying a voltage between the pair of electrodes of the organic luminescence device to cause phosphorescence from the organic compound layer (luminescence function layer) containing the metal coordination compound.

[0054] According to the present invention, there is further provided an image display apparatus including the organic luminescence device and means for supplying electrical signals to the organic luminescence device.

[0055] These and other objects, features and advantages of the present invention will become more apparent upon a consideration of the following description of the preferred embodiments of the present invention taken in conjunction with the accompanying drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

[0056] **FIGS. 1A, 1B** and **1**C are respectively a schematic sectional view of a layer structure of an organic luminescence device.

[0057] **FIG. 2** is a schematic perspective view of an organic luminescence device of a single matrix-type used in Example 3 appearing hereinafter.

[0058] **FIG. 3** is a waveform diagram of a driving signal employed in Example 3.

[0059] **FIG. 4A** shows luminescence spectrum diagram of a phenylpyrimidine-based Ir complex ($Ir(ppy)_3$), and **FIG. 4B** shows a luminescence spectrum diagram of a thienylpyridine-based Ir complex ($Ir(thpy)_3$).

[0060] **FIG. 5** shows a luminescence spectrum diagram of 2-benzylpyridine Ir complex used in Example 10.

DESCRIPTION OF THE PREFERRED EMBODIMENTS

[0061] In the case where a luminescence layer for an organic EL device is formed of a carrier transporting host material and a phosphorescent guest material, a process of emission of light (phosphorescence) may generally involve the following steps:

[0062] (1) transport of electron and hole within a luminescence layer,

[0063] (2) formation of exciton of the host material,

[0064] (3) transmission of excited energy between host material molecules,

[0065] (4) transmission of excited energy from the host material molecule to the guest material molecule,

[0066] (5) formation of triplet exciton of the guest material, and

[0067] (6) emission of light (phosphorescence) caused during transition from the triplet excited state to the ground state of the guest material.

[0068] In the above steps, desired energy transmission and luminescence may generally be caused based on various quenching and competition.

[0069] In order to improve a luminescence efficiency of the EL device, a luminescence center material per se is required to provide a higher yield of luminescence quantum. In addition thereto, an efficient energy transfer between host material molecules and/or between host material molecule and guest material molecule is also an important factor.

[0070] Further, the above-described luminescent deterioration in energized state may presumably relate to the luminescent center material per se or an environmental change thereof by its ambient molecular structure.

[0071] The metal coordination compound represented by the above formula (1) according to the present invention causes phosphorescence (luminescence) and is assumed to have a lowest excited state comprising a triplet excited state liable to cause metal-to-ligand charge transfer (MLCT* state) or π-π^* state as a ligand-centered triplet excited state. The phosphorescent emission of light (phosphorescence) is caused to occur during the transition from the MLCT* state or π-π^* state to the ground state.

[0072] The metal coordination compound of formula (1) according to the present invention has been found to provide a higher phosphorescence yield of at least 0.01 and a shorter phosphorescence life of 1-100 μsec.

[0073] The shorter phosphorescence life is necessary to provide a resultant EL device with a higher luminescence efficiency. This is because the longer phosphorescence life increases molecules placed in their triplet excited state which is a waiting state for phosphorescence, thus lowering the resultant luminescence efficiency particularly at a higher current density.

[0074] Accordingly, the metal coordination compound of formula (1) according to the present invention is a suitable luminescent material for an organic EL device with a higher phosphorescence yield and a shorter phosphorescence life.

[0075] Further, due to the shorter phosphorescence life, molecules of the metal coordination compound of formula (1) have a shorter time period wherein they stay in the triplet excited state, i.e. a higher energy state, thus providing the resultant EL device with improved durability and less deterioration in device characteristic. In this regard, the metal coordination compound according to the present invention has been substantiated to exhibit excellent stability of luminance as shown in Examples described hereinafter.

[0076] The organic luminescence device according to the present invention has a layer structure wherein an organic compound layer (luminescence function layer) comprising the metal coordination compound of the formula (1) s sandwiched between a pair of oppositely disposed electrodes as shown in **FIGS. 1A** to **1**C. The organic luminescence device exhibits phosphorescence from the organic compound layer by applying a voltage between the pair of electrodes.

[0077] The metal coordination compound of the formula (1) according to the present invention used in the organic luminescence device (EL device) as a luminescence function material, particularly a luminescent material may be roughly classified into the following two compounds:

[0078] (1) a metal coordination compound having a molecular structure containing the same species of plural (two or three) ligands, and

[0079] (2) a metal coordination compound having a molecular structure containing different species of plural ligands.

[0080] In the present invention, it is possible to appropriately design a molecular structure of metal coordination compound so as to provide a stably high luminescence efficiency and maximum luminescence wavelength by using ligands different in structure in either case (of the above (1) and (2)).

[0081] In the case (1) using the same species of ligands, it is possible to provide a smaller half-width of luminescence spectrum and a higher color purity.

[0082] Further, in the case (2) using different species of ligands, it is possible to employ different two ligands for the metal coordination compound of the formula (1), thus imparting a plurality of functions (multi-function) to the metal coordination compound based on the respective features of the ligands. The impartition of multi-function is a characteristic feature of the use of different species of ligands. Particularly, in the case where the metal coordination compound having different species of ligands is used in an organic EL device, incorporation into the metal coordination compound of different species of ligands capable of imparting controlled luminescence and current characteristics to the EL device is very advantageous to the EL device since device characteristics of the EL device is largely affected by not only the luminescence characteristic but also the current characteristic.

[0083] An organic luminescence device using a phosphorescence material having different ligand structure has been described in M. E. Thompson et al., "Electrophotophorescent Organic Light Emitting Diodes" (Conference record of the 20th International Display Research Conference), pp. 337-340 (2000). In this document, Ir coordination com-

pounds having luminescent ligands containing a phenylpyridine skeleton or a thienylpyridine skeleton and an additional ligand containing an acetylacetone skeleton. By using the Ir coordination compounds, a synthesis yield is improved without lowering a luminescence characteristic compared with Ir complex having (identical) three ligands of phenylpyridine (tris-acetylacetonato-Ir complex).

[0084] However, the tris-acetylacetonato-Ir complex exhibits no or a slight phosphorescence and has no carrier (hole/electron) transport performance.

[0085] In the above document, the acetylacetone ligand ((acac)ligand) is employed for the purpose of improving the synthesis yield without impairing the luminescence performance as described above, thus failing to positively suggesting improvement in device characteristics of an organic EL device.

[0086] According to our experiment, the device characteristics of the organic EL device have been found to be improved by imparting functions described below to different two ligands constituting a different ligand structure.

[0087] In order to determine an inherent feature of a ligand, at first, a metal coordination compound having one metal connected with the same species of ligands is synthesized and subjected to measurement of its characteristics (affected by a combination of the metal with the ligands), such as a (maximum) luminescence wavelength (emission wavelength), a luminescence yield, an electron transfer performance, a hole transfer performance and a thermal stability.

[0088] In this regard, in order to determine the luminescence characteristics including the luminescence wavelength and yield, a characteristic of luminescence molecules placed in a minimum excited state is an important factor.

[0089] As described above, the minimum excited state of the metal coordination compound of the formula (1) according to the present invention is the MLCT excited state or the ligand-centered excited state. In the case of a phosphorescence material, the MLCT excited state is generally advantageous thereto since the phosphorescence material (placed in the MLCT excited state) has a higher luminescence transition probability and a stronger luminescence performance in many cases.

[0090] Based on a combination of ligands and a (central) metal, a resultant metal coordination compound is determined whether its excited state is the MLCT excited state or the ligand-centered excited state.

[0091] Herein, the terms "MLCT (metal to ligand charge transfer) excited state" refers to an excited state formed by localization of electron orbit of molecules constituting the metal coordination compound towards the ligand side, thus causing a transfer of one electron side, thus causing a transfer of one electron from the metal to the ligand. On the other hand, the term "ligand-centered excited state" refers to an excited state formed within the ligands without being directly affected by the metal at the time of excitation. Generally, an electron is excited from bonding π-orbital to nonbonding π-orbital. Accordingly, the ligand-centered excited state is also called "π-π^* excited state".

[0092] The carrier (hole/electron) transfer performance or ability may, e.g., be evaluated by measuring an increased amount of a current value flowing between a pair of electrodes sandwiching an organic compound layer (luminescence function layer) containing dispersed metal coordination compound having the same species of ligands, relative to that in the case of using no metal coordination compound.

[0093] Further, it is possible to determine whether H the organic compound layer is an electron transport layer or a hole transport layer by comparing a current characteristic of an organic luminescence device having a multi-layer structure including two organic compound layers sandwiching a luminescence layer therebetween with respect to various organic compounds constituting organic compound layers.

[0094] As described above, it becomes possible to characterize ligands constituting the metal coordination compound of the present invention by appropriately changing a combination of the metal and ligands.

[0095] Then, in order to improve the luminescence characteristics of a metal coordination compound having a different ligand structure, we presume that it is preferred to smoothly effect excited energy transition between ligands placed in their excited states to cause luminescence based on a particular ligand while minimizing the number of luminescent ligand.

[0096] More specifically, when a metal coordination compound having three ligands including one luminescent ligand is placed in excited state, excited energy is transferred from two ligands to one luminescent ligand, thus allowing a monochromatic luminescent color and an increased color purity. Further, it is expected that the use of one luminescent ligand decreases a probability of occurrence of energy transition between spatially adjacent molecules of the metal coordination compound, thus resulting in a decrease in quenching or deactivated energy.

[0097] Accordingly, in the present invention, a preferred class of combinations of a plurality of ligands may include:

[0098] (a) a combination of ligands including at least one ligand capable of being placed in the MLCT excited state,

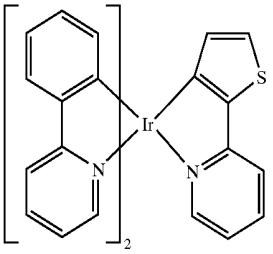
[0099] (b) a combination of ligands including both of a luminescent ligand and a carrier transport ligand,

[0100] (c) a combination of ligands including a first ligand providing a longer maximum luminescence wavelength $\lambda 1$ (i.e., smaller excited energy) and a second ligand providing a shorter maximum luminescence wavelength $\lambda 2$ ($<\lambda 1$) (i.e., larger excited energy) wherein the number of the first ligand is smaller than that of the second ligand, and

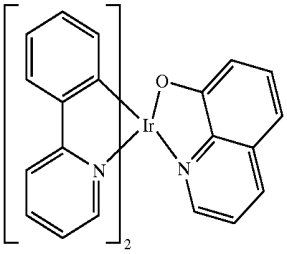
[0101] (d) a combination of ligands including a stronger luminescent ligand and a weaker luminescent ligand wherein the number of the stronger luminescent ligand is smaller than that of the weaker luminescent ligand.

[0102] The above ligand combinations (a) to (d) will be described below more specifically by taking Ir complexes as an example.

Formula 41



Formula 42



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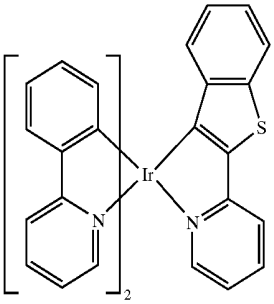
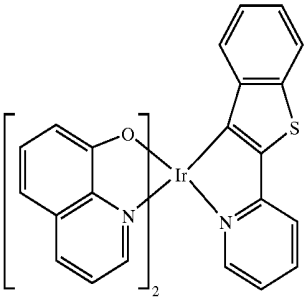
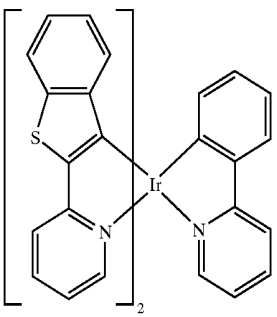


Formula 44



Formula 45



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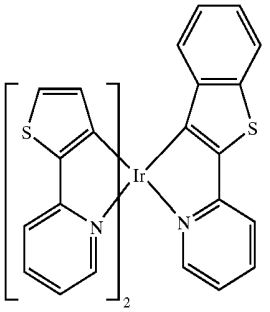
Formula 46



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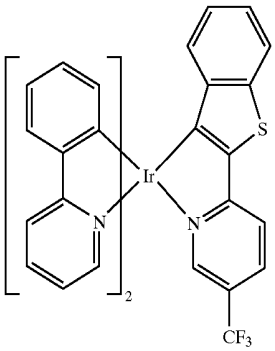
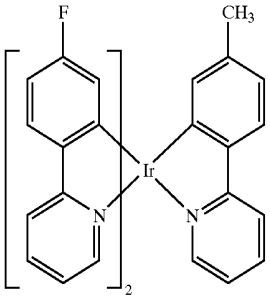
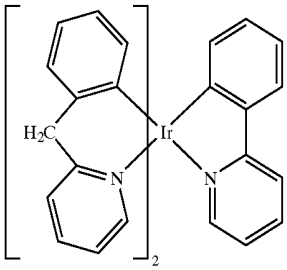


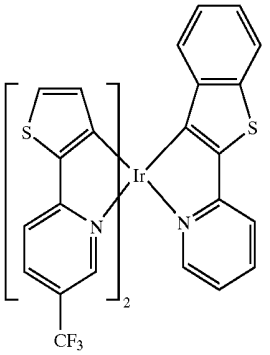
Formula 48



Formula 49



Formula 50



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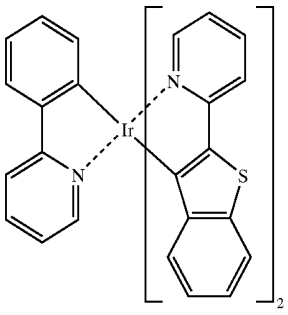
Formula 51



[0103] The metal coordination compounds having the above structural formulas 41 to 51 may be classified as follows.

Combination	Formula
(a)	41, 42, 43
(b)	44, 45
(c)	46, 47, 48, 49
(d)	48, 50

[0104] The metal coordination compounds of the formulas 41-51 includes those which can be embraced in a plurality of the combinations (a)-(d).

[0105] Combination (a)

[0106] The metal coordination compound of the formula 41 has two phenylpyridine ligands and one thienylpyridine ligand respectively connected to Ir (center metal). When the metal coordination compound is excited, the phenylpyridine ligands are placed in the MLCT excited state and the thienylpyridine ligand is placed in the ligand-centered excited state.

[0107] The excited state (MLCT or ligand-centered excited state) is identified based on shapes of emission spectra of Ir complex having three phenylpyridine skeletons ($Ir(ppy)_3$) and Ir complex having three thienylpyridine skeletons ($Ir(thpy)_3$), diagrams of which are shown in **FIGS. 4A and 4B**, respectively.

[0108] Referring to **FIG. 4A**, $Ir(ppy)_3$ shows no peak other than a main peak. On the other hand, as shown in **FIG. 4B**, $Ir(thpy)_3$ shows a sub-peak (or shoulder) other than a main peak on the longer wavelength side. This sub-peak is resulting from a vibrational level of an aromatic ligand and thus is not observed in the case of the MLCT excited state.

[0109] In the case of phosphorescence, compared with the case of the ligand-centered excited state, the case of the MLCT excited state is considerably allowed to exhibit transition with luminescence (phosphorescence) from the excited state to the ground state. Further, a probability of such transition is higher than that of transition with no radiation, thus generally providing a higher phosphorescence yield.

[0110] $Ir(ppy)_3$ shows no sub-peak as in the case of $Ir(thpy)_3$, thus being identified to be placed in the MLCT excited state.

[0111] Accordingly, in the case of the metal coordination compound of the formula 41, when the phenylpyridine ligand is first excited, the excitation energy is not quenched or deactivated but is quickly intramolecular-transferred to the thienylpyridine ligand to place the thienylpyridine ligand in an excited state. This is because the triplet energy level of phenylpyridine is higher than that of thienylpyridine.

[0112] Even in both the case of an organic EL device and the case of photoluminescence (PL) in a photo-excitation solution, luminescence at 550 nm resulting from the thienylpyridine ligand is observed.

[0113] Similarly, the 8-quinolinol ligand in the metal coordination compound of the formula 42 and the benzothienylpyridine ligand in the metal coordination compound of the formula 43 are ligands placed in the ligand-centered excited state. In these cases of using the metal coordination compounds of the formula 42 and 43, luminescences resulting from the 8 -quinolinol ligand and the benzothienylpyridine ligand as a longer-wavelength luminescent ligand are observed, respectively.

[0114] In the case where a ligand in the MLCT excited state provides a longer maximum luminescence wavelength, luminescence resulting from the ligand in the MLCT excited state.

[0115] Further, for example, in the case of the metal coordination compound of the formula 48 having the 4-fluorophenylpyridine ligand and the 4 -methylphenylpyridine ligand both in the MLCT excited state, quenching with no luminescence is not readily caused to occur.

[0116] The maximum luminescence wavelength of the 4-fluorophenylpyridine is shorter than (i.e., excitation energy level thereof is higher than) that of the 4-methylphenylpyridine. Accordingly, even when either ligand is excited, excitation energy is intramolecular-transferred to the 4-methylphenyl-pyridine ligand with a lower excitation energy level to cause luminescence resulting from the 4-methylphenylpyridine. The metal coordination compound of the formula 48 is thus placed in the MLCT excited state, thus not readily causing quenching with no radiation to allow a high-efficiency luminescence.

[0117] Accordingly, when the metal coordination compound of the present invention has a different ligand structure including a ligand capable of being placed in the MLCT excited state, it becomes possible to effect intramolecular energy transition at a high efficiency, thus ensuring a high phosphorescence yield.

[0118] Combination (b)

[0119] The metal coordination compound of the formula 44 has the f-quinolinol ligand as an electron transport ligand and the benzothienylpyridine ligand as a luminescent ligand. When the metal coordination compound of the formula 44 is dispersed in the luminescence layer **12** of the organic EL device shown in **FIG. 1C**, it is possible to improve a luminescence efficiency compared with the case of using a metal coordination compound having the same ligand structure comprising three f-quinolinol ligands (i.e., tris-8-quinolinolato-Ir complex).

[0120] Further, when compared with an organic EL device using no luminescence material (the metal coordination compound of the formula 44 in this case), the organic EL

device using the metal coordination compound of the formula 44 effectively improves a resultant current density under application of an identical voltage. This may be attributable to such a mechanism that the electron transport 8-quinolinol ligand allows supply of electrons to the luminescence layer (into which carrier electrons are ordinarily to readily injected) by dispersing the metal coordination compound of the formula 44 in the luminescence layer, thus forming excitons by combination with holes to ensure efficient luminescence based on the luminescence benzothienylpyridine ligand.

[0121] The benzothienylpyridine ligand also exhibits a hole transport performance. In the metal coordination compound of the formula 45, the benzothienylpyridine ligand has a hole transport function.

[0122] Combination (c)

[0123] The metal coordination compound of the formula 46 has the thienylpyridine ligand and the benzothienylpyridine ligand.

[0124] An Ir complex having three thienylpyridine ligands and an Ir complex having three benzothienyl-pyridine ligands causes phosphorescence at maximum luminescence wavelengths of 550 nm and 600 nm, respectively. Accordingly, the latter Ir complex has a longer maximum luminescence wavelength and a smaller lowest excitation energy (triplet energy in this case). Luminescence resulting from the benzothienyl-pyridine ligand is observed both in the case of an organic EL device using the metal coordination compound of the formula 46 and in the case of PL (photoluminescence) in a photo-excitation solution thereof.

[0125] When an organic EL device shown in **FIG. 1C** is prepared by using the metal coordination compound of the formula 46, it is possible to obtain a high luminescence efficiency. This may be attributable to such a mechanism that, compared with a metal coordination compound having (identical) three benzothienylpyridine ligands (luminescent ligands), the number of luminescent ligand in the metal coordination compound of the formula 46 is ⅓ of the metal coordination compound having three benzothienyl-pyridine ligands to decrease a probability of formation of quenching path with no luminescence by intermolecular interaction with ambient molecules.

[0126] Accordingly, it becomes possible to realize a high luminescence efficiency by decreasing the number of the longer-wavelength luminescent ligand relative to that of the shorter-wavelength luminescent ligand.

[0127] With respect to the metal coordination compound of the formula 49, the benzylpyridine ligand exhibits a blue luminescence characteristic (emission peak wavelength: 480 nm) and the phenylpyridine ligand exhibits a green luminescence characteristic (emission peak wavelength: 515 nm).

[0128] As a result, excitation energy is concentrated on the phenylpyridine ligand, thus ensuring stable luminescence resulting from the phenylpyridine ligand.

[0129] Combination (d)

[0130] The metal coordination compound of the formula 50 has the thienyl-4-trifluoromethylpyridine ligand and the benzothienylpyridine ligand.

[0131] According to our experiment as to luminescence characteristic in a solution (e.g., in deoxidized toluene), a photo-excitation phosphorescence yield in the solution of an Ir complex having three thienyl-4-trifluoromethylpyridine ligands is smaller than that of an Ir complex having three benzothienylpyridine ligands. Accordingly, the benzothienylpyridine ligand is a relatively stronger luminescent ligand compared with the thienyl-4-trifluoromethylpyridine ligand. Further, the former ligand also provides a relatively longer maximum luminescence wavelength (i.e., a relatively lower excitation energy level). For this reason, luminescence from the metal coordination compound of the formula 49 is one resulting from the benzo-thienylpyridine ligands based on intramolecular energy transfer.

[0132] By using the metal coordination compound of the formula 49 in a luminescence layer **12** for an organic EL device shown in **FIG. 1C, a** high luminescence efficiency is achieved.

[0133] Accordingly, it is possible to improve a luminescence efficiency by decreasing the number (1 in this case) of stronger luminescent ligand and longer-wavelength luminescent ligand.

[0134] As described above, the metal coordination compound of the present invention satisfying at least one of the above-mentioned combinations (a) to (d) effectively functions as a luminescence function material and provides a resultant organic EL device with a high luminescence efficiency. In the present invention, it is generally expected to increase the luminescence efficiency by ca. 20% when compared with the case of using a metal coordination compound having identical three luminescent ligands, but a degree of increase in luminescence efficiency may vary depending on species of the metal and ligands.

[0135] The above-mentioned high-efficiency organic luminescence device may be applicable to various products requiring energy saving and high luminescence, such as light sources for a display apparatus, illumination apparatus, printers, etc., and a backlight for a liquid crystal display apparatus.

[0136] When the organic luminescence device of the present invention is used as an image display apparatus, it becomes possible to provide flat-panel displays with advantages such as a good energy saving performance, high visibility, and lightweight properties.

[0137] The organic luminescence device of the present invention is also prepared in a single matrix-type display device using intersecting stripe electrodes at right angles or an active matrix-type display device including a matrix of pixels each provided with, e.g., at least one TFT (thin film transistor), such as amorphous TFT or polycrystalline TFT.

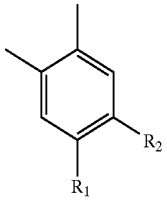
[0138] When the organic luminescence device of the present invention is used as a light source for a printer, e.g., as a laser light source for a laser beam printer, independently addressable elements are arranged in an array and a photosensitive drum is subjected to desired exposure, thus effecting image formation. By the use of the organic luminescence device of the present invention, it becomes possible to considerably reduce the apparatus size (volume).

[0139] With respect to the illumination apparatus and the backlight, it is expected that the organic luminescence device of the present invention effectively exhibits an excellent energy saving effect.

[0140] Hereinbelow, specific examples of the metal coordination compound of the formula (1) according to the present invention will be shown in Table 1. The metal coordination compound of the present invention is however not restricted to these specific examples.

[0141] In Table 1, abbreviations Ph to P_2 for CyN1, CyN2, CyN3, CyC1, CyC2 and CyC3 and those O to CR2 for -X- represent the following divalent groups, respectively.

Ph:



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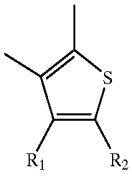

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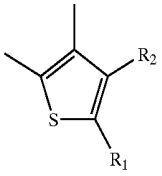

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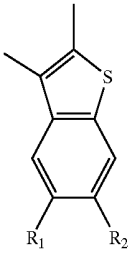

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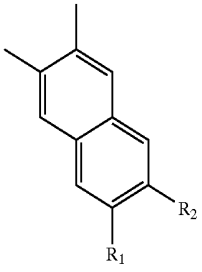

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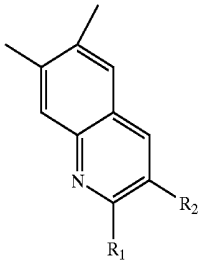

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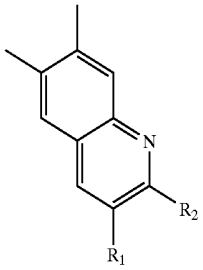

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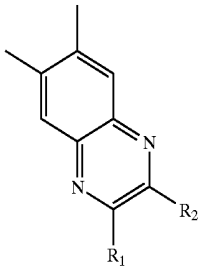
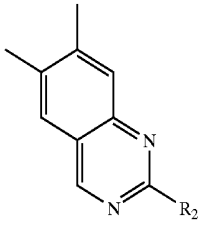
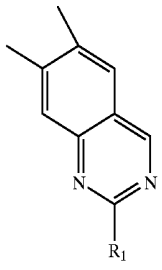


Qz1:



Qz2:



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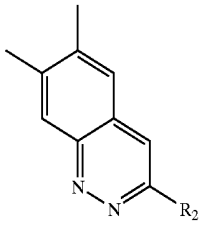
Cn1:



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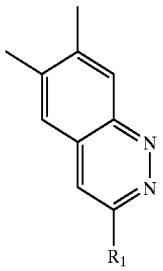
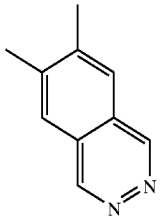


Pz:



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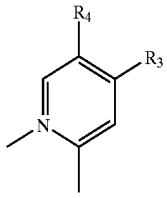
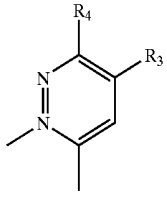
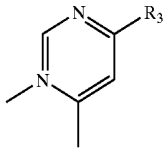


Pd:



Py1:



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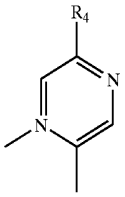
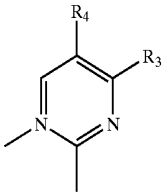
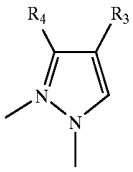
Pa:



Py2:



Pz:



O:

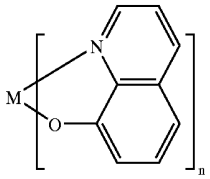
S:

NR:

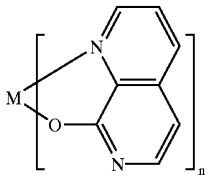
CO:

CR_2:

[0142] Further, formulas (11) to (14) corresponding to the partial structure ML'n as the formula (5) (including CyN4 being 8-quinolinol skeleton or its derivative) shown as L' in Table 1 for convenience represent the following structures, respectively.



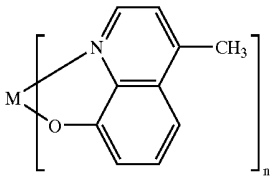
(11)



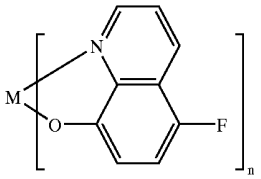
(12)

-continued

(13)



(14)



[0143] Further, Example Compounds Nos. 215 to 218 and 746 include an acetylacetone ligand as L' for another ligand of the formula (6).

TABLE 1

				L									
					X								
No	M	m	n	CyN1	/	CyC1	R1	R2	R3	R4	R5	R6	L'
1	Ir	3	0	Pr	O	Ph	H	H	H	H			
2	Ir	3	0	Pr	O	Tn1	H	H	H	H			
3	Ir	3	0	Pr	O	Tn2	H	H	H	H			
4	Ir	3	0	Pr	O	Tn3	H	H	H	H			
5	Ir	3	0	Pr	O	Qn1	H	H	H	H			
6	Ir	3	0	Pr	O	Qn2	H	H	H	H			
7	Ir	3	0	Pr	O	Qx	H	H	H	H			
8	Ir	3	0	Pr	O	Qz1	—	H	H	H			
9	Ir	3	0	Pr	O	Qz2	H	—	H	H			
10	Ir	3	0	Pr	O	Cn1	—	H	H	H			
11	Ir	3	0	Pr	O	Cn2	H	—	H	H			
12	Ir	3	0	Pr	O	Pz	—	—	H	H			
13	Ir	3	0	Pr	S	Ph	H	H	H	H			
14	Ir	3	0	Pr	S	Tn1	H	H	H	H			
15	Ir	3	0	Pr	S	Tn2	H	H	H	H			
16	Ir	3	0	Pr	S	Tn3	H	H	H	H			
17	Ir	3	0	Pr	S	Qn1	H	H	H	H			
18	Ir	3	0	Pr	S	Qn2	H	H	H	H			
19	Ir	3	0	Pr	S	Qx	H	H	H	H			
20	Ir	3	0	Pr	S	Qz1	—	H	H	H			
21	Ir	3	0	Pr	S	Qz2	H	—	H	H			
22	Ir	3	0	Pr	S	Cn1	—	H	H	H			
23	Ir	3	0	Pr	S	Cn2	H	—	H	H			
24	Ir	3	0	Pr	S	Pz	—	—	H	H			
25	Ir	3	0	Pr	NR	Ph	H	H	H	H	H		
26	Ir	3	0	Pr	NR	Tn1	H	H	H	H	H		
27	Ir	3	0	Pr	NR	Tn2	H	H	H	H	H		
28	Ir	3	0	Pr	NR	Tn3	H	H	H	H	H		
29	Ir	3	0	Pr	NR	Qn1	H	H	H	H	H		
30	Ir	3	0	Pr	NR	Qn2	H	H	H	H	H		
31	Ir	3	0	Pr	NR	Qx	H	H	H	H	H		
32	Ir	3	0	Pr	NR	Qz1	—	H	H	H	H		
33	Ir	3	0	Pr	NR	Qz2	H	—	H	H	H		
34	Ir	3	0	Pr	NR	Cn1	—	H	H	H	H		
35	Ir	3	0	Pr	NR	Cn2	H	—	H	H	H		
36	Ir	3	0	Pr	NR	Pz	—	—	H	H	H		
37	Ir	3	0	Pr	CO	Ph	H	H	H	H			
38	Ir	3	0	Pr	CO	Tn1	H	H	H	H			
39	Ir	3	0	Pr	CO	Tn2	H	H	H	H			
40	Ir	3	0	Pr	CO	Tn3	H	H	H	H			
41	Ir	3	0	Pr	CO	Qn1	H	H	H	H			

TABLE 1-continued

42	Ir	3	0	Pr	CO	Qn2	H	H	H	H		
43	Ir	3	0	Pr	CO	Qx	H	H	H	H		
44	Ir	3	0	Pr	CO	Qz1	—	H	H	H		
45	Ir	3	0	Pr	CO	Qz2	H	—	H	H		
46	Ir	3	0	Pr	CO	Cn1	—	H	H	H		
47	Ir	3	0	Pr	CO	Cn2	H	—	H	H		
48	Ir	3	0	Pr	CO	Pz	—	—	H	H		
49	Ir	3	0	Pr	CR2	Ph	H	H	H	H	H	H
50	Ir	3	0	Pr	CR2	Tn1	H	H	H	H	H	H
51	Ir	3	0	Pr	CR2	Tn2	H	H	H	H	H	H
52	Ir	3	0	Pr	CR2	Tn3	H	H	H	H	H	H
53	Ir	3	0	Pr	CR2	Qn1	H	H	H	H	H	H
54	Ir	3	0	Pr	CR2	Qn2	H	H	H	H	H	H
55	Ir	3	0	Pr	CR2	Qx	H	H	H	H	H	H
56	Ir	3	0	PR	CR2	Qz1	—	H	H	H	H	H
57	Ir	3	0	Pr	CR2	Qx2	H	—	H	H	H	H
58	Ir	3	0	Pr	CR2	Cn1	—	H	H	H	H	H
59	Ir	3	0	Pr	CR2	Cn2	H	—	H	H	H	H
60	Ir	3	0	Pr	CR2	Pz	—	—	H	H	H	H
61	Ir	3	0	Pd	O	Ph	H	H	H	H		
62	Ir	3	0	Pd	O	Tn1	H	H	H	H		
63	Ir	3	0	Pd	O	Tn2	H	H	H	H		
64	Ir	3	0	Pd	O	Tn3	H	H	H	H		
65	Ir	3	0	Pd	S	Ph	H	H	H	H		
66	Ir	3	0	Pd	S	Tn1	H	H	H	H		
67	Ir	3	0	Pd	S	Tn2	H	H	H	H		
68	Ir	3	0	Pd	S	Tn3	H	H	H	H		
69	Ir	3	0	Pd	NR	Ph	H	H	H	H	H	
70	Ir	3	0	Pd	NR	Tn1	H	H	H	H	H	
71	Ir	3	0	Pd	NR	Tn2	H	H	H	H	H	
72	Ir	3	0	Pd	NR	Tn3	H	H	H	H	H	
73	Ir	3	0	Pd	CO	Ph	H	H	H	H		
74	Ir	3	0	Pd	CO	Tn1	H	H	H	H		
75	Ir	3	0	Pd	CO	Tn2	H	H	H	H		
76	Ir	3	0	Pd	CO	Tn3	H	H	H	H		
77	Ir	3	0	Pd	CR2	Ph	H	H	H	H	H	H
78	Ir	3	0	Pd	CR2	Tn1	H	H	H	H	H	H
79	Ir	3	0	Pd	CR2	Tn2	H	H	H	H	H	H
80	Ir	3	0	Pd	CR2	Tn3	H	H	H	H	H	H
81	Ir	3	0	Pr1	O	Ph	H	H	H	—		
82	Ir	3	0	Pr1	O	Tn1	H	H	H	—		
83	Ir	3	0	Pr1	O	Tn2	H	H	H	—		
84	Ir	3	0	Pr1	O	Tn3	H	H	H	—		
85	Ir	3	0	Pr1	S	Ph	H	H	H	—		
86	Ir	3	0	Pr1	S	Tn1	H	H	H	—		
87	Ir	3	0	Pr1	S	Tn2	H	H	H	—		
88	Ir	3	0	Pr1	S	Tn3	H	H	H	—		
89	Ir	3	0	Pr1	NR	Ph	H	H	H	—	H	
90	Ir	3	0	Pr1	NR	Tn1	H	H	H	—	H	
91	Ir	3	0	Pr1	NR	Tn2	H	H	H	—	H	
92	Ir	3	0	Pr1	NR	Tn3	H	H	H	—	H	
93	Ir	3	0	Pr1	CO	Ph	H	H	H	—		
94	Ir	3	0	Pr1	CO	Tn1	H	H	H	—		
95	Ir	3	0	Pr1	CO	Tn2	H	H	H	—		
96	Ir	3	0	Pr1	CO	Tn3	H	H	H	—		
97	Ir	3	0	Pr1	CR2	Ph	H	H	H	—	H	H
98	Ir	3	0	Pr1	CR2	Tn1	H	H	H	—	H	H
99	Ir	3	0	Pr1	CR2	Tn2	H	H	H	—	H	H
100	Ir	3	0	Pr1	CR2	Tn3	H	H	H	—	H	H
101	Ir	3	0	Pa	O	Ph	H	H	—	H		
102	Ir	3	0	Pa	O	Tn1	H	H	—	H		
103	Ir	3	0	Pa	O	Tn2	H	H	—	H		
104	Ir	3	0	Pa	O	Tn3	H	H	—	H		
105	Ir	3	0	Pa	S	Ph	H	H	—	H		
106	Ir	3	0	Pa	S	Tn1	H	H	—	H		
107	Ir	3	0	Pa	S	Tn2	H	H	—	H		
108	Ir	3	0	Pa	S	Tn3	H	H	—	H		
109	Ir	3	0	Pa	NR	Ph	H	H	—	H	H	
110	Ir	3	0	Pa	NR	Tn1	H	H	—	H	H	
111	Ir	3	0	Pa	NR	Tn2	H	H	—	H	H	
112	Ir	3	0	Pa	NR	Tn3	H	H	—	H	H	
113	Ir	3	0	Pa	CO	Ph	H	H	—	H		
114	Ir	3	0	Pa	CO	Tn1	H	H	—	H		
115	Ir	3	0	Pa	CO	Tn2	H	H	—	H		
116	Ir	3	0	Pa	CO	Tn3	H	H	—	H		
117	Ir	3	0	Pa	CR2	Ph	H	H	—	H	H	H

TABLE 1-continued

118	Ir	3	0	Pa	CR2	Tn1	H	H	—	H	H	H
119	Ir	3	0	Pa	CR2	Tn2	H	H	—	H	H	H
120	Ir	3	0	Pa	CR2	Tn3	H	H	—	H	H	H
121	Ir	3	0	Pr2	O	Ph	H	H	H	H		
122	Ir	3	0	Pr2	O	Tn1	H	H	H	H		
123	Ir	3	0	Pr2	O	Tn2	H	H	H	H		
124	Ir	3	0	Pr2	O	Tn3	H	H	H	H		
125	Ir	3	0	Pr2	S	Ph	H	H	H	H		
126	Ir	3	0	Pr2	S	Tn1	H	H	H	H		
127	Ir	3	0	Pr2	S	Tn2	H	H	H	H		
128	Ir	3	0	Pr2	S	Tn3	H	H	H	H		
129	Ir	3	0	Pr2	NR	Ph	H	H	H	H	H	
130	Ir	3	0	Pr2	NR	Tn1	H	H	H	H	H	
131	Ir	3	0	Pr2	NR	Tn2	H	H	H	H	H	
132	Ir	3	0	Pr2	NR	Tn3	H	H	H	H	H	
133	Ir	3	0	Pr2	CO	Ph	H	H	H	H		
134	Ir	3	0	Pr2	CO	Tn1	H	H	H	H		
135	Ir	3	0	Pr2	CO	Tn2	H	H	H	H		
136	Ir	3	0	Pr2	CO	Tn3	H	H	H	H		
137	Ir	3	0	Pr2	CR2	Ph	H	H	H	H	H	
138	Ir	3	0	Pr2	CR2	Tn1	H	H	H	H	H	
139	Ir	3	0	Pr2	CR2	Tn2	H	H	H	H	H	
140	Ir	3	0	Pr2	CR2	Tn3	H	H	H	H	H	
141	Ir	3	0	Pz	O	Ph	H	H	H	H		
142	Ir	3	0	Pz	O	Tn1	H	H	H	H		
143	Ir	3	0	Pz	O	Tn2	H	H	H	H		
144	Ir	3	0	Pz	O	Tn3	H	H	H	H		
145	Ir	3	0	Pz	S	Ph	H	H	H	H		
146	Ir	3	0	Pz	S	Tn1	H	H	H	H		
147	Ir	3	0	Pz	S	Tn2	H	H	H	H		
148	Ir	3	0	Pz	S	Tn3	H	H	H	H		
149	Ir	3	0	Pz	NR	Ph	H	H	H	H	H	
150	Ir	3	0	Pz	NR	Tn1	H	H	H	H	H	
151	Ir	3	0	Pz	NR	Tn2	H	H	H	H	H	
152	Ir	3	0	Pz	NR	Tn3	H	H	H	H	H	
153	Ir	3	0	Pz	CO	Ph	H	H	H	H		
154	Ir	3	0	Pz	CO	Tn1	H	H	H	H		
155	Ir	3	0	Pz	CO	Tn2	H	H	H	H		
156	Ir	3	0	Pz	CO	Tn3	H	H	H	H		
157	Ir	3	0	Pz	CR2	Ph	H	H	H	H	H	H
158	Ir	3	0	Pz	CR2	Tn1	H	H	H	H	H	H
159	Ir	3	0	Pz	CR2	Tn2	H	H	H	H	H	H
160	Ir	3	0	Pz	CR2	Tn3	H	H	H	H	H	H
161	Ir	3	0	Pr	NR	Ph	H	H	H	H	phenyl	
162	Ir	3	0	Pr	NR	Ph	H	H	H	H	naphthyl	
163	Ir	3	0	Pr	NR	Ph	H	H	H	H	—CH3	
164	Ir	3	0	Pr	NR	Ph	H	H	H	H	—C4H9	
165	Ir	3	0	Pr	CR2	Qn1	H	H	H	H	—CH3	—CH3
166	Ir	3	0	Pr	CR2	Qn2	H	H	H	H	—C4H9	—C4H9
167	Ir	3	0	Pr	CR2	Qx	H	H	H	H	H	—CH3
168	Ir	3	0	Pr	CR2	Qz1	—	H	H	H	H	—C4H9
169	Ir	3	0	Pr	CR2	Ph	H	H	H	CF3	H	
170	Ir	3	0	Pr	CR2	Ph	H	CF3	H	H	H	
171	Ir	3	0	Pr	CR2	Ph	H	H	H	CH3	H	
172	Ir	3	0	Pr	CR2	Ph	H	H	CH3	H	H	
173	Ir	3	0	Pr	CR2	Qn1	H	H	H	OCF3	H	H
174	Ir	3	0	Pr	CR2	Qn2	H	OC2H5	H	H	H	H
175	Ir	3	0	Pr	CR2	Qx	H	H	H	OC2H5	H	H
176	Ir	3	0	Pr	CR2	Qz1	—	H	COOC2H5	H	H	H
177	Ir	3	0	Pr	O	Ph	H	H	H	CF3	—	
178	Ir	3	0	Pr	O	Ph	H	CF3	H	H	—	
179	Ir	3	0	Pr	NR2	Ph	H	H	H	CH3	H	
180	Ir	3	0	Pr	NR2	Ph	H	H	CH3	H	H	
181	Ir	3	0	Pr	NR2	Qn1	H	H	H	OCF3	H	—
182	Ir	3	0	Pr	CO	Qn2	H	OC2H5	H	H	—	—
183	Ir	3	0	Pr	CO	Qx	H	H	H	OC2H5	—	—
184	Ir	3	0	Pr	CO	Qz1	—	H	COOC2H5	H	—	—
185	Rh	3	0	Pr	CO	Ph	H	H	H	H		
186	Rh	3	0	Pr	CO	Tn1	H	H	H	H		
187	Rh	3	0	Pr	CR2	Tn2	H	H	H	H	H	H
188	Rh	3	0	Pr	CR2	Tn3	H	H	H	H	H	H
189	Rh	3	0	Pr	O	Qn1	H	H	H	H		
190	Rh	3	0	Pr	O	Qn2	H	H	H	H		
191	Rh	3	0	Pr	S	Qx	H	H	H	H		
192	Rh	3	0	Pr	S	Qz1	—	H	H	H		
193	Rh	3	0	Pr	NR	Qz2	H	—	H	H	H	

TABLE 1-continued

194	Rh	3	0	Pr	NR	Cnl	H	H		H		H				
195	Pd	2	0	Pr	CO	Ph	H	H		H		H				
196	Pd	2	0	Pr	CO	Tn1	H	H		H		H				
197	Pd	2	0	Pr	CR2	Tn2	H	H		H		H		H		
198	Pd	2	0	Pr	CR2	Tn3	H	H		H		H		H		
199	Pd	2	0	Pr	O	Qn1	H	H		H		H				
200	Pd	2	0	Pr	O	Qn2	H	H		H		H				
201	Pd	2	0	Pr	S	Qx	H	H		H		H				
202	Pd	2	0	Pr	S	Qz1	—	H		H		H				
203	Pd	2	0	Pr	NR	Qz2	H	—		H		H		H		
204	Pd	2	0	Pr	NR	Cn1	—	H		H		H		H		
205	Pt	2	0	Pr	CO	Ph	H	H		H		H				
206	Pt	2	0	Pr	CO	Tn1	H	H		H		H				
207	Pt	2	0	Pr	CR2	Tn2	H	H		H		H		H		
208	Pt	2	0	Pr	CR2	Tn3	H	H		H		H		H		
209	Pt	2	0	Pr	O	Qn1	H	H		H		H				
210	Pt	2	0	Pr	O	Qn2	H	H		H		H				
211	Pt	2	0	Pr	S	Qx	H	H		H		H				
212	Pt	2	0	Pr	S	Qz1	—	H		H		H				
213	Pt	2	0	Pr	NR	Qz2	H	—		H		H		H		
214	Pt	3	0	Pr	NR	Cn1	—	H		H		H		H		
215	Ir	2	0	Pr	CR2	Ph	H	H		H		H		H		H	CH3—CO—CH—CO—CH3
216	Ir	2	0	Pr	CR2	Tn1	H	H		H		H		H		H	CH3—CO—CH—CO—CH3
217	Ir	2	0	Pr	CO	Tn2	H	H		H		H					CH3—CO—CH—CO—CH3
218	Ir	2	0	Pr	CO	Tn3	H	H		H		H					CH3—CO—CH—CO—CH3

				L													
				CyN1 or CyN2	X	CyC1 or CyC2	R1	R2	R3	R4	R5	R6	CyN3	CyC3	R1	L' R2	R3	R4
No	M	m	n															
219	Ir	2	1	Pr	O	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
220	Ir	2	1	Pr	O	Ph	H	H	H	H			Pr	Ph	H	H	H	H
221	Ir	2	1	Pr	O	Ph	H	H	H	H			Py1	Ph	H	H	H	—
222	Ir	2	1	Pr	O	Ph	H	H	H	H			Pr	Ph	CH3	H	H	H
223	Ir	2	1	Pr	O	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
224	Ir	2	1	Pr	O	Ph	H	H	H	H			Py1	Ph	H	H	H	—
225	Ir	2	1	Pr	CO	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
226	Ir	2	1	Pr	CO	Ph	H	H	H	H			Pr	Ph	H	H	H	H
227	Ir	2	1	Pr	CO	Ph	H	H	H	H			Py1	Ph	H	H	H	—
228	Ir	2	1	Pr	CO	Ph	H	H	H	H			Pr	Ph	CH3	H	H	H
229	Ir	2	1	Pr	CO	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
230	Ir	2	1	Pr	CO	Ph	H	H	H	H			Py1	Ph	H	H	H	—
231	Ir	2	1	Pr	NR	Ph	H	H	H	H	CH3		Pr	Tn1	H	H	H	H
232	Ir	2	1	Pr	NR	Ph	H	H	H	H	CH3		Pr	Ph	H	H	H	H
233	Ir	2	1	Pr	NR	Ph	H	H	H	H	CH3		Py1	Ph	H	H	H	—
234	Ir	2	1	Pr	NR	Ph	H	H	H	H	CH3		Pr	Ph	CF3	H	H	H
235	Ir	2	1	Pr	NR	Ph	H	H	H	H	CH3		Pr	Tn1	H	H	H	H
236	Ir	2	1	Pr	NR	Ph	H	H	H	H	CH3		Py1	Ph	H	H	H	—
237	Ir	2	1	Pr	NR	Tn1	H	H	H	H	C2H5		Pr	Tn1	H	H	H	H
238	Ir	2	1	Pr	NR	Tn1	H	H	H	H	C2H5		Pr	Ph	H	H	H	H
239	Ir	2	1	Pr	NR	Tn1	H	H	H	H	C2H5		Py1	Ph	H	H	H	—
240	Ir	2	1	Pr	NR	Qn1	H	H	H	H	C2H5		Pr	Ph	F	H	H	H
241	Ir	2	1	Pr	NR	Qn1	H	H	H	H	C2H5		Pr	Tn1	H	H	H	H
242	Ir	2	1	Pr	NR	Qn1	H	H	H	H	C2H5		Py1	Ph	H	H	H	—
243	Pt	1	1	Pr	O	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
244	Pt	1	1	Pr	O	Ph	H	H	H	H			Pr	Ph	H	H	H	H
245	Pt	1	1	Pr	O	Ph	H	H	H	H			Py1	Ph	H	H	H	—
246	Pt	1	1	Pr	O	Ph	H	H	H	H			Pr	Ph	CH3	H	H	H
247	Pt	1	1	Pr	O	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
248	Pt	1	1	Pr	O	Ph	H	H	H	H			Py1	Ph	H	H	H	—
249	Pt	1	1	Pr	CO	Ph	H	H	H	H			Pr	Tn1	H	H	H	H
250	Pt	1	1	Pr	CO	Ph	H	H	H	H			Pr	Ph	H	H	H	H
251	Pt	1	1	Pr	CO	Ph	H	H	H	H			Py1	Ph	H	H	H	—
252	Pt	1	1	Pr	CO	Ph	H	H	H	H			Pr	Ph	CH3	H	H	H

TABLE 1-continued

253	Pt	1	1	Pr	CO	Ph	H	H	H	H		Pr	Tn1	H	H	H	H
254	Pt	1	1	Pr	CO	Ph	H	H	H	H		Py1	Ph	H	H	H	—
255	Pt	1	1	Pr	NR	Ph	H	H	H	H	CH3	Pr	Tn1	H	H	H	H
256	Pt	1	1	Pr	NR	Ph	H	H	H	H	CH3	Pr	Ph	H	H	H	H
257	Pt	1	1	Pr	NR	Ph	H	H	H	H	CH3	Py1	Ph	H	H	H	—
258	Pt	1	1	Pr	NR	Ph	H	H	H	H	CH3	Pr	Ph	CF3	H	H	H
259	Pt	1	1	Pr	NR	Ph	H	H	H	H	CH3	Pr	Tn1	H	H	H	H
260	Pt	1	1	Pr	NR	Ph	H	H	H	H	CH3	Py1	Ph	H	H	H	—
261	Pt	1	1	Pr	NR	Tn1	H	H	H	H	C2H5	Pr	Tn1	H	H	H	H
262	Pt	1	1	Pr	NR	Tn1	H	H	H	H	C2H5	Pr	Ph	H	H	H	H
263	Pt	1	1	Pr	NR	Tn1	H	H	H	H	C2H5	Py1	Ph	H	H	H	—
264	Pt	1	1	Pr	NR	Qn1	H	H	H	H	C2H5	Pr	Ph	F	H	H	H
265	Pt	1	1	Pr	NR	Qn1	H	H	H	H	C2H5	Pr	Tn1	H	H	H	H
266	Pt	1	1	Pr	NR	Qn1	H	H	H	H	C2H5	Py1	Ph	H	H	H	—
267	Ir	2	1	Pr	—	Ph	F	H	H	H		Pr	Ph	CH3	H	H	H
268	Ir	2	1	Pr	—	Ph	F	F	H	H		Pr	Ph	H	H	H	H
269	Ir	2	1	Pr	—	Ph	F	H	H	H		Pr	Ph	CF3	H	H	H
270	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Tn1	H	H	H	H
271	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Tn2	H	H	H	H
272	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Tn3	H	H	H	H
273	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Np	H	H	H	H
274	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Qn1	H	H	H	H
275	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Qn2	H	H	H	H
276	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Qx	H	H	H	H
277	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Qz1	—	H	H	H
278	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Qz2	H	—	H	H
279	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Cn1	—	H	H	H
280	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Cn2	H	—	H	H
281	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Pz	—	—	H	H
282	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Ph	CH3	H	H	H
283	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	Ph	H	CF3	H	H
284	Ir	2	1	Pr	—	Ph	H	H	H	H		Pr	tn3	H	H	H	CF3
285	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Tn1	H	H	H	H
286	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Tn2	H	H	H	H
287	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Tn3	H	H	H	H
288	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Np	H	H	H	H
289	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Qn1	H	H	H	H
290	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Qn2	H	H	H	H
291	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Qx	H	H	H	H
292	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Qx1	—	H	H	H
293	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Qx2	H	—	H	H
294	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Cn1	—	H	H	H
295	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Cn2	H	—	H	H
296	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Pz	—	—	H	H
297	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Ph	CH3	H	H	H
298	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	Ph	H	CF3	H	H
299	Ir	1	2	Pr	—	Ph	H	H	H	H		Pr	tn3	H	H	H	CF3
300	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Tn3	H	H	H	H
301	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Np	H	H	H	H
302	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Qn1	H	H	H	H
303	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Qn2	H	H	H	H
304	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Qx	H	H	H	H
305	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Qz1	—	H	H	H
306	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Qz2	H	—	H	H
307	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Cn1	—	H	H	H
308	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Cn2	H	—	H	H
309	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Pz	—	—	H	H
310	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Ph	CH3	H	H	H
311	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	Ph	H	CF3	H	H
312	Ir	2	1	Pr	—	Tn1	H	H	H	H		Pr	tn3	H	H	H	CF3
313	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Tn3	H	H	H	H
314	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Np	H	H	H	H
315	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Qn1	H	H	H	H
316	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Qn2	H	H	H	H
317	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Qx	H	H	H	H
318	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Qz1	—	H	H	H
319	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Qz1	H	—	H	H
320	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Cn1	—	H	H	H
321	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Cn2	H	—	H	H
322	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Pz	—	—	H	H
323	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Ph	CH3	H	H	H
324	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	Ph	H	CF3	H	H
325	Ir	1	2	Pr	—	Tn1	H	H	H	H		Pr	tn3	H	H	H	CF3
326	Ir	2	1	Py1	—	Ph	H	H	H	H		Pr	Tn1	H	H	H	H
327	Ir	2	1	Py1	—	Ph	H	H	H	H		Pr	Tn1	H	H	H	H
328	Ir	2	1	Py1	—	Ph	H	H	H	H		Pr	Tn3	H	H	H	H

TABLE 1-continued

329	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Np	H	H	H	H
330	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Qn1	H	H	H	H
331	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Qn2	H	H	H	H
332	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Qx	H	H	H	H
333	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Qz1	—	H	H	H
334	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Qz2	H	—	H	H
335	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Cn1	—	H	H	H
336	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Cn2	H	—	H	H
337	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Pz	—	—	H	H
338	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Ph	CH3	H	H	H
339	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	Ph	H	CF3	H	H
340	Ir	2	1	Py1	—	Ph	H	H	H	H	Pr	tn3	H	H	H	CF3
341	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Tn1	H	H	H	H
342	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Tn2	H	H	H	H
343	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Tn3	H	H	H	H
344	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Np	H	H	H	H
345	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Qn1	H	H	H	H
346	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Qn2	H	H	H	H
347	Ir	1	2	Py1	—	Ph	H	H	H	H	Pr	Qx	H	H	H	H
348	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Qz1	—	H	H	H
349	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Qz2	H	—	H	H
350	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Cn1	—	H	H	H
351	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Cn2	H	—	H	H
352	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Pz	—	—	H	H
353	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Ph	CH3	H	H	H
354	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	Ph	H	CF3	H	H
355	Ir	1	2	Py1	—	Pr	H	H	H	H	Pr	tn3	H	H	H	CF3
356	Ir	2	1	Py1	—	Ph	H	H	H	H	Pz	Tn1	H	H	H	H
357	Ir	2	1	Py1	—	Ph	H	H	H	H	Pz	Tn2	H	H	H	H
358	Ir	2	1	Py1	—	Ph	H	H	H	H	Pz	Tn3	H	H	H	H
359	Ir	2	1	Py1	—	Ph	H	H	H	H	Pa	Np	H	H	—	H
360	Ir	2	1	Py1	—	Ph	H	H	H	H	Pa	Qn1	H	H	—	H
361	Ir	2	1	Py1	—	Ph	H	H	H	H	Pa	Qn2	H	H	—	H
362	Ir	2	1	Py1	—	Ph	H	H	H	H	Py2	Qx	H	H	H	H
363	Ir	2	1	Py1	—	Ph	H	H	H	H	Py2	Qz1	H	—	H	H
364	Ir	2	1	Py1	—	Ph	H	H	H	H	Py2	Qz2	H	—	H	H
365	Ir	2	1	Py1	—	Ph	H	H	H	H	Py1	Cn1	—	H	H	H
366	Ir	2	1	Py1	—	Ph	H	H	H	H	Py1	Cn2	H	—	H	H
367	Ir	2	1	Py1	—	Ph	H	H	H	H	Py1	Pz	—	—	H	H
368	Ir	2	1	Py1	—	Ph	H	H	H	H	Py2	Ph	CH3	H	H	H
369	Ir	2	1	Py1	—	Ph	H	H	H	H	Py2	Ph	H	CF3	H	H
370	Ir	2	1	Py1	—	Ph	H	H	H	H	Py2	tn3	H	H	H	CF3
371	Ir	2	1	Pr	—	Ph	H	H	H	H	formula 11					
372	Ir	2	1	Pr	—	Ph	H	H	H	H	formula 12					
373	Ir	2	1	Pr	—	Ph	H	H	H	H	formula 13					
374	Ir	2	1	Pr	—	Ph	H	H	H	H	formula 14					
375	Ir	2	1	Pr	—	Tn1	H	H	H	H	formula 11					
376	Ir	2	1	Pr	—	Tn1	H	H	H	H	formula 12					
377	Ir	2	1	Pr	—	Tn1	H	H	H	H	formula 13					
378	Ir	2	1	Pr	—	Tn1	H	H	H	H	formula 14					
379	Ir	2	1	Pr	—	Tn3	H	H	H	H	formula 11					
380	Ir	2	1	Pr	—	Tn3	H	H	H	H	formula 12					
381	Ir	2	1	Pr	—	Tn3	H	H	H	H	formula 13					
382	Ir	2	1	Pr	—	Tn3	H	H	H	H	formula 14					
383	Ir	2	1	Pr	—	Np	H	H	H	H	formula 11					
384	Ir	2	1	Pr	—	Np	H	H	H	H	formula 12					
385	Ir	2	1	Pr	—	Np	H	H	H	H	formula 13					
386	Ir	2	1	Pr	—	Np	H	H	H	H	formula 14					
387	Ir	2	1	Pr	—	Qn2	H	H	H	H	formula 11					
388	Ir	2	1	Pr	—	Qn2	H	H	H	H	formula 12					
389	Ir	2	1	Pr	—	Qn2	H	H	H	H	formula 13					
390	Ir	2	1	Pr	—	Qn2	H	H	H	H	formula 14					
391	Ir	2	1	Py1	—	Ph	H	H	H	—	formula 11					
392	Ir	2	1	Py1	—	Ph	H	H	H	—	formula 12					
393	Ir	2	1	Py1	—	Ph	H	H	H	—	formula 13					
394	Ir	2	1	Py1	—	Ph	H	H	H	—	formula 14					
395	Ir	2	1	Py2	—	Ph	H	H	H	H	formula 11					
396	Ir	2	1	Py2	—	Ph	H	H	H	H	formula 12					
397	Ir	2	1	Py2	—	Ph	H	H	H	H	formula 13					
398	Ir	2	1	Py2	—	Ph	H	H	H	H	formula 14					
399	Ir	2	1	Pz	—	Ph	H	H	H	H	formula 11					
400	Ir	2	1	Pz	—	Ph	H	H	H	H	formula 12					
401	Ir	2	1	Pz	—	Ph	H	H	H	H	formula 13					
402	Ir	2	1	Pz	—	Ph	H	H	H	H	formula 14					
403	Ir	2	1	Pa	—	Ph	H	H	—	H	formula 11					
404	Ir	2	1	Pa	—	Ph	H	H	—	H	formula 12					

TABLE 1-continued

405	Ir	2	1	Pa	—	Ph	H	H	—	H			formula 13			
406	Ir	2	1	pa	—	Ph	H	H	—	H			formula 14			
407	Ir	1	2	Pr	—	Ph	H	H	H	H			formula 11			
408	Ir	1	2	Pr	—	Ph	H	H	H	H			formula 12			
409	Ir	1	2	Pr	—	Ph	H	H	H	H			formula 13			
410	Ir	1	2	Pr	—	Ph	H	H	H	H			formula 14			
411	Ir	1	2	Pr	—	Tn1	H	H	H	H			formula 11			
412	Ir	1	2	Pr	—	Tn1	H	H	H	H			formula 12			
413	Ir	1	2	Pr	—	Tn1	H	H	H	H			formula 13			
414	Ir	1	2	Pr	—	Tn1	H	H	H	H			formula 14			
415	Ir	1	2	Pr	—	Tn3	H	H	H	H			formula 11			
416	Ir	1	2	Pr	—	Tn3	H	H	H	H			formula 12			
417	Ir	1	2	Pr	—	Tn3	H	H	H	H			formula 13			
418	Ir	1	2	Pr	—	Tn3	H	H	H	H			formula 14			
419	Ir	1	2	Pr	—	Np	H	H	H	H			formula 11			
420	Ir	1	2	Pr	—	Np	H	H	H	H			formula 12			
421	Ir	1	2	Pr	—	Np	H	H	H	H			formula 13			
422	Ir	1	2	Pr	—	Np	H	H	H	H			formula 14			
423	Ir	1	2	Pr	—	Qn2	H	H	H	H			formula 11			
424	Ir	1	2	Pr	—	Qn2	H	H	H	H			formula 12			
425	Ir	1	2	Pr	—	Qn2	H	H	H	H			formula 13			
426	Ir	1	2	Pr	—	Qn2	H	H	H	H			formula 14			
427	Ir	1	2	Py1	—	Ph	H	H	H	—			formula 11			
428	Ir	1	2	Py1	—	Ph	H	H	H	—			formula 12			
429	Ir	1	2	Py1	—	Ph	H	H	H	—			formula 13			
430	Ir	1	2	Py1	—	Ph	H	H	H	—			formula 14			
431	Ir	1	2	Py2	—	Ph	H	H	H	H			formula 11			
432	Ir	1	2	Py2	—	Ph	H	H	H	H			formula 12			
433	Ir	1	2	Py2	—	Ph	H	H	H	H			formula 13			
434	Ir	1	2	Py2	—	Ph	H	H	H	H			formula 14			
435	Ir	1	2	Pz	—	Ph	H	H	H	H			formula 11			
436	Ir	1	2	Pz	—	Ph	H	H	H	H			formula 12			
437	Ir	1	2	Pz	—	Ph	H	H	H	H			formula 13			
438	Ir	1	2	Pz	—	Ph	H	H	H	H			formula 14			
439	Ir	1	2	Pa	—	Ph	H	H	—	H			formula 11			
440	Ir	1	2	Pa	—	Ph	H	H	—	H			formula 12			
441	Ir	1	2	Pa	—	Ph	H	H	—	H			formula 13			
442	Ir	1	2	Pa	—	Ph	H	H	—	H			formula 14			
443	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Tn1	H	H	H	H
444	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Tn2	H	H	H	H
445	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Tn3	H	H	H	H
446	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Np	H	H	H	H
447	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Qn1	H	H	H	H
448	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Qn2	H	H	H	H
449	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Qx	H	H	H	H
450	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Qz1	—	H	H	H
451	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Qz2	H	—	H	H
452	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Cn1	—	H	H	H
453	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Cn2	H	—	H	H
454	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Pz	—	—	H	H
455	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Ph	CH3	H	H	H
456	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	Ph	H	CF3	H	H
457	Rh	2	1	Pr	—	Ph	H	H	H	H	Pr	tn3	H	H	H	CF3
458	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Tn1	H	H	H	H
459	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Tn2	H	H	H	H
460	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Tn3	H	H	H	H
461	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Np	H	H	H	H
462	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Qn1	H	H	H	H
463	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Qn2	H	H	H	H
464	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Qx	H	H	H	H
465	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Qz1	—	H	H	H
466	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Qz2	H	—	H	H
467	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Cn1	—	H	H	H
468	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Cn2	H	—	H	H
469	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Pz	—	—	H	H
470	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Ph	CH3	H	H	H
471	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	Ph	H	CF3	H	H
472	Rh	1	2	Pr	—	Ph	H	H	H	H	Pr	tn3	H	H	H	CF3
473	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Tn3	H	H	H	H
474	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Np	H	H	H	H
475	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Qn1	H	H	H	H
476	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Qn2	H	H	H	H
477	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Qx	H	H	H	H
478	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Qz1	—	H	H	H
479	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Qz2	H	—	H	H
480	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Cn1	—	H	H	H

TABLE 1-continued

481	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Qn2	H	—	H	H
482	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Pz	—	—	H	H
483	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Ph	CH3	H	H	H
484	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	Ph	H	CF3	H	H
485	Rh	2	1	Pr	—	Tn1	H	H	H	H	Pr	tn3	H	H	H	CF3
486	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Tn3	H	H	H	H
487	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Np	H	H	H	H
488	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Qn1	H	H	H	H
489	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Qn2	H	H	H	H
490	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Qx	H	H	H	H
491	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Qz1	—	H	H	H
492	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Qz2	H	—	H	H
493	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Cr1	—	H	H	H
494	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Cn2	H	—	H	H
495	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Pz	—	—	H	H
496	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Ph	CH3	H	H	H
497	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	Ph	H	CF3	H	H
498	Rh	1	2	Pr	—	Tn1	H	H	H	H	Pr	tn3	H	H	H	CF3
499	Rh	2	1	Pr	—	Ph	H	H	H	H	formula 11					
500	Rh	2	1	Pr	—	Ph	H	H	H	H	formula 12					
501	Rh	2	1	Pr	—	Ph	H	H	H	H	formula 13					
502	Rh	2	1	Pr	—	Ph	H	H	H	H	formula 14					
503	Rh	2	1	Pr	—	Tn1	H	H	H	H	formula 11					
504	Rh	2	1	Pr	—	Tn1	H	H	H	H	formula 12					
505	Rh	2	1	Pr	—	Tn1	H	H	H	H	formula 13					
506	Rh	2	1	Pr	—	Tn1	H	H	H	H	formula 14					
507	Rh	2	1	Pr	—	Tn3	H	H	H	H	formula 11					
508	Rh	2	1	Pr	—	Tn3	H	H	H	H	formula 12					
509	Rh	2	1	Pr	—	Tn3	H	H	H	H	formula 13					
510	Rh	2	1	Pr	—	Tn3	H	H	H	H	formula 14					
511	Rh	2	1	Pr	—	Np	H	H	H	H	formula 11					
512	Rh	2	1	Pr	—	Np	H	H	H	H	formula 12					
513	Rh	2	1	Pr	—	Np	H	H	H	H	formula 13					
514	Rh	2	1	Pr	—	Np	H	H	H	H	formula 14					
515	Rh	2	1	Pr	—	Qn2	H	H	H	H	formula 11					
516	Rh	2	1	Pr	—	Qn2	H	H	H	H	formula 12					
517	Rh	2	1	Pr	—	Qn2	H	H	H	H	formula 13					
518	Rh	2	1	Pr	—	Qn2	H	H	H	H	formula 14					
519	Rh	2	1	Py1	—	Ph	H	H	H	—	formula 11					
520	Rh	2	1	Py1	—	Ph	H	H	H	—	formula 12					
521	Rh	2	1	Py1	—	Ph	H	H	H	—	formula 13					
522	Rh	2	1	Py1	—	Ph	H	H	H	—	formula 14					
523	Rh	2	1	Py2	—	Ph	H	H	H	H	formula 11					
524	Rh	2	1	Py2	—	Ph	H	H	H	H	formula 12					
525	Rh	2	1	Py2	—	Ph	H	H	H	H	formula 13					
526	Rh	2	1	Py2	—	Ph	H	H	H	H	formula 14					
527	Rh	2	1	Pz	—	Ph	H	H	H	H	formula 11					
528	Rh	2	1	Pz	—	Ph	H	H	H	H	formula 12					
529	Rh	2	1	Pz	—	Ph	H	H	H	H	formula 13					
530	Rh	2	1	Pz	—	Ph	H	H	H	H	formula 14					
531	Rh	2	1	Pa	—	Ph	H	H	—	H	formula 11					
532	Rh	2	1	Pa	—	Ph	H	H	—	H	formula 12					
533	Rh	2	1	Pa	—	Ph	H	H	—	H	formula 13					
534	Rh	2	1	Pa	—	Ph	H	H	—	H	formula 14					
535	Rh	1	2	Pr	—	Ph	H	H	H	H	formula 11					
536	Rh	1	2	Pr	—	Ph	H	H	H	H	formula 12					
537	Rh	1	2	Pr	—	Ph	H	H	H	H	formula 13					
538	Rh	1	2	Pr	—	Ph	H	H	H	H	formula 14					
539	Rh	1	2	Pr	—	Tn1	H	H	H	H	formula 11					
540	Rh	1	2	Pr	—	Tn1	H	H	H	H	formula 12					
541	Rh	1	2	Pr	—	Tn1	H	H	H	H	formula 13					
542	Rh	1	2	Pr	—	Tn1	H	H	H	H	formula 14					
543	Rh	1	2	Pr	—	Tn3	H	H	H	H	formula 11					
544	Rh	1	2	Pr	—	Tn3	H	H	H	H	formula 12					
545	Rh	1	2	Pr	—	Tn3	H	H	H	H	formula 13					
546	Rh	1	2	Pr	—	Tn3	H	H	H	H	formula 14					
547	Rh	1	2	Pr	—	Np	H	H	H	H	formula 11					
548	Rh	1	2	Pr	—	Np	H	H	H	H	formula 12					
549	Rh	1	2	Pr	—	Np	H	H	H	H	formula 13					
550	Rh	1	2	Pr	—	Np	H	H	H	H	formula 14					
551	Rh	1	2	Pr	—	Qn2	H	H	H	H	formula 11					
552	Rh	1	2	Pr	—	Qn2	H	H	H	H	formula 12					
553	Rh	1	2	Pr	—	Qn2	H	H	H	H	formula 13					
554	Rh	1	2	Pr	—	Qn2	H	H	H	H	formula 14					
555	Rh	1	2	Py1	—	Ph	H	H	H	—	formula 11					
556	Rh	1	2	Py1	—	Ph	H	H	H	—	formula 12					

TABLE 1-continued

557	Rh	1	2	Py1	—	Ph	H	H	H	—				formula 13		
558	Rh	1	2	Py1	—	Ph	H	H	H	—				formula 14		
559	Rh	1	2	Py2	—	Ph	H	H	H	H				formula 11		
560	Rh	1	2	Py2	—	Ph	H	H	H	H				formula 12		
561	Rh	1	2	Py2	—	Ph	H	H	H	H				formula 13		
562	Rh	1	2	Py2	—	Ph	H	H	H	H				formula 14		
563	Rh	1	2	Pz	—	Ph	H	H	H	H				formula 11		
564	Rh	1	2	Pz	—	Ph	H	H	H	H				formula 12		
565	Rh	1	2	Pz	—	Ph	H	H	H	H				formula 13		
566	Rh	1	2	Pz	—	Ph	H	H	H	H				formula 14		
567	Rh	1	2	Pa	—	Ph	H	H	—	H				formula 11		
568	Rh	1	2	Pa	—	Ph	H	H	—	H				formula 12		
569	Rh	1	2	Pa	—	Ph	H	H	—	H				formula 13		
570	Rh	1	2	Pa	—	Ph	H	H	—	H				formula 14		
571	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Tn1	H	H	H	H
572	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Tn2	H	H	H	H
573	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Tn3	H	H	H	H
574	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Np	H	H	H	H
575	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Qn1	H	H	H	H
576	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Qn2	H	H	H	H
577	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Qx	H	H	H	H
578	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Qz1	—	H	H	H
579	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Qz2	H	—	H	H
580	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Cn1	—	H	H	H
581	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Cn2	H	—	H	H
582	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Pz	—	—	H	H
583	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Ph	CH3	H	H	H
584	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	Ph	H	CF3	H	H
585	Pt	1	1	Pr	—	Ph	H	H	H	H	Pr	tn3	H	H	H	CF3
586	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Tn3	H	H	H	H
587	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Np	H	H	H	H
588	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qn1	H	H	H	H
589	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qn2	H	H	H	H
590	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qx	H	H	H	H
591	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qz1	—	H	H	H
592	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qz2	H	—	H	H
593	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Cn1	—	H	H	H
594	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Cn2	H	—	H	H
595	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Pz	—	—	H	H
596	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Ph	CH3	H	H	H
597	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	Ph	H	CF3	H	H
598	Pt	1	1	Pr	—	Tn1	H	H	H	H	Pr	tn3	H	H	H	CF3
599	Pt	1	1	Pr	—	Ph	H	H	H	H				formula 11		
600	Pt	1	1	Pr	—	Ph	H	H	H	H				formula 12		
601	Pt	1	1	Pr	—	Ph	H	H	H	H				formula 13		
602	Pt	1	1	Pr	—	Ph	H	H	H	H				formula 14		
603	Pt	1	1	Pr	—	Tn1	H	H	H	H				formula 11		
604	Pt	1	1	Pr	—	Tn1	H	H	H	H				formula 12		
605	Pt	1	1	Pr	—	Tn1	H	H	H	H				formula 13		
606	Pt	1	1	Pr	—	Tn1	H	H	H	H				formula 14		
607	Pt	1	1	Pr	—	Tn3	H	H	H	H				formula 11		
608	Pt	1	1	Pr	—	Tn3	H	H	H	H				formula 12		
609	Pt	1	1	Pr	—	Tn3	H	H	H	H				formula 13		
610	Pt	1	1	Pr	—	Tn3	H	H	H	H				formula 14		
611	Pt	1	1	Pr	—	Np	H	H	H	H				formula 11		
612	Pt	1	1	Pr	—	Np	H	H	H	H				formula 12		
613	Pt	1	1	Pr	—	Np	H	H	H	H				formula 13		
614	Pt	1	1	Pr	—	Np	H	H	H	H				formula 14		
615	Pt	1	1	Pr	—	Qn2	H	H	H	H				formula 11		
616	Pt	1	1	Pr	—	Qn2	H	H	H	H				formula 12		
617	Pt	1	1	Pr	—	Qn2	H	H	H	H				formula 13		
618	Pt	1	1	Pr	—	Qn2	H	H	H	H				formula 14		
619	Pt	1	1	Py1	—	Ph	H	H	H	—				formula 11		
620	Pt	1	1	Py1	—	Ph	H	H	H	—				formula 12		
621	Pt	1	1	Py1	—	Ph	H	H	H	—				formula 13		
622	Pt	1	1	Py1	—	Ph	H	H	H	—				formula 14		
623	Pt	1	1	Py2	—	Ph	H	H	H	H				formula 11		
624	Pt	1	1	Py2	—	Ph	H	H	H	H				formula 12		
625	Pt	1	1	Py2	—	Ph	H	H	H	H				formula 13		
626	Pt	1	1	Py2	—	Ph	H	H	H	H				formula 14		
627	Pt	1	1	Pz	—	Ph	H	H	H	H				formula 11		
628	Pt	1	1	Pz	—	Ph	H	H	H	H				formula 12		
629	Pt	1	1	Pz	—	Ph	H	H	H	H				formula 13		
630	Pt	1	1	Pz	—	Ph	H	H	H	H				formula 14		
631	Pt	1	1	Pa	—	Ph	H	H	H	—				formula 11		
632	Pt	1	1	Pa	—	Ph	H	H	H	—				formula 12		

TABLE 1-continued

633	Pt	1	1	Pa	—	Ph	H	H	H	—				formula 13		
634	Pt	1	1	Pa	—	Ph	H	H	H	—				formula 14		
635	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Tn1	H	H	H	H
636	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Tn2	H	H	H	H
637	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Tn3	H	H	H	H
638	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Np	H	H	H	H
639	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Qn1	H	H	H	H
640	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Qn2	H	H	H	H
641	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Qx	H	H	H	H
642	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Qz1	—	H	H	H
643	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Oz2	H	—	H	H
644	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Cn1	—	H	H	H
645	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Cn2	H	—	H	H
646	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Pz	—	—	H	H
647	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Ph	CH3	H	H	H
648	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	Ph	H	CF3	H	H
649	Pd	1	1	Pr	—	Ph	H	H	H	H	Pr	tn3	H	H	H	CF3
650	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Tn3	H	H	H	H
651	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Np	H	H	H	H
652	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qn1	H	H	H	H
653	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qn2	H	H	H	H
654	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qx	H	H	H	H
655	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qz1	—	H	H	H
656	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Qz2	H	—	H	H
657	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Cn1	—	H	H	H
658	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Cn2	H	—	H	H
659	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Pz	—	—	H	H
660	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Ph	CH3	H	H	H
661	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	Ph	H	CF3	H	H
662	Pd	1	1	Pr	—	Tn1	H	H	H	H	Pr	tn3	H	H	H	CF3
663	Pd	1	1	Pr	—	Ph	H	H	H	H				formula 11		
664	Pd	1	1	Pr	—	Ph	H	H	H	H				formula 12		
665	Pd	1	1	Pr	—	Ph	H	H	H	H				formula 13		
666	Pd	1	1	Pr	—	Ph	H	H	H	H				formula 14		
667	Pd	1	1	Pr	—	Tn1	H	H	H	H				formula 11		
668	Pd	1	1	Pr	—	Tn1	H	H	H	H				formula 12		
669	Pd	1	1	Pr	—	Tn1	H	H	H	H				formula 13		
670	Pd	1	1	Pr	—	Tn1	H	H	H	H				formula 14		
671	Pd	1	1	Pr	—	Tn3	H	H	H	H				formula 11		
672	Pd	1	1	Pr	—	Tn3	H	H	H	H				formula 12		
673	Pd	1	1	Pr	—	Tn3	H	H	H	H				formula 13		
674	Pd	1	1	Pr	—	Tn3	H	H	H	H				formula 14		
675	Pd	1	1	Pr	—	Np	H	H	H	H				formula 11		
676	Pd	1	1	Pr	—	Np	H	H	H	H				formula 12		
677	Pd	1	1	Pr	—	Np	H	H	H	H				formula 13		
678	Pd	1	1	Pr	—	Np	H	H	H	H				formula 14		
679	Pd	1	1	Pr	—	Qn2	H	H	H	H				formula 11		
680	Pd	1	1	Pr	—	Qn2	H	H	H	H				formula 12		
681	Pd	1	1	Pr	—	Qn2	H	H	H	H				formula 13		
682	Pd	1	1	Pr	—	Qn2	H	H	H	H				formula 14		
683	Pd	1	1	Py1	—	Ph	H	H	H	—				formula 11		
684	Pd	1	1	Py1	—	Ph	H	H	H	—				formula 12		
685	Pd	1	1	Py1	—	Ph	H	H	H	—				formula 13		
686	Pd	1	1	Py1	—	Ph	H	H	H	—				formula 14		
687	Pd	1	1	Py2	—	Ph	H	H	H	H				formula 11		
688	Pd	1	1	Py2	—	Ph	H	H	H	H				formula 12		
689	Pd	1	1	Py2	—	Ph	H	H	H	H				formula 13		
690	Pd	1	1	Py2	—	Ph	H	H	H	H				formula 14		
691	Pd	1	1	Pz	—	Ph	H	H	H	H				formula 11		
692	Pd	1	1	Pz	—	Ph	H	H	H	H				formula 12		
693	Pd	1	1	Pz	—	Ph	H	H	H	H				formula 13		
694	Pd	1	1	Pz	—	Ph	H	H	H	H				formula 14		
695	Pd	1	1	Pa	—	Ph	H	H	—	H				formula 11		
696	Pd	1	1	Pa	—	Ph	H	H	—	H				formula 12		

TABLE 1-continued

697	Pd	1	1	Pa	—	Ph	H	H	—	H			formula 13
698	Pd	1	1	Pa	—	Ph	H	H	—	H			formula 14

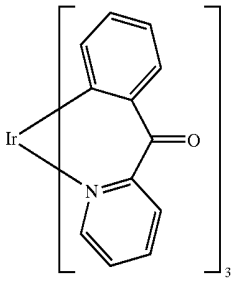
				L								
No	M	m	n	CyN1	X	CyC1	R1	R2	R3	R4	R5	R6	L'
699	Ir	2	0	Pr	CR2	Ph	H	H	H	H	F	F	CH3—CO—CH—CO—CH3
700	Ir	3	0	Pr	CR2	Ph	H	H	H	H	F	F	

[0144] Hereinbelow, the present invention will be described more specifically based on Examples with reference to the drawing.

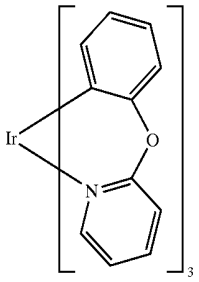
EXAMPLES 1 AND 2

[0145] In these examples, the following metal coordination compounds of formula (1) (Ex. Comp. Nos. 37 and 1) were used in respective luminescence layers for Examples 1 and 2 respectively.

[0146] Ex. Comp. No. 37



[0147] Ex. Comp. No. 1



[0148] Each of organic luminescence devices having a structure including four organic (compound) layers (luminescence function layers) shown in **FIG. 1C** were prepared in the following manner.

[0149] On a 1.1 mm-thick glass substrate (transparent substrate **15**), a 100 nm-thick film (transparent electrode **14**) of ITO (indium tin oxide) was formed by sputtering, followed by patterning to have an (opposing) electrode area of 3 mm^2.

[0150] On the ITO-formed substrate, four organic layers and two metal electrode layers shown below were successively formed by vacuum (vapor) deposition using resistance heating in a vacuum chamber (10^{-4} Pa).

[0151] Organic layer **1** (hole transport layer **13**) (50 nm): α-NPD

[0152] Organic layer **2** (luminescence layer **12**) (40 nm): CBP: metal coordination compound of formula (1) (93:7 by weight) (co-vacuum deposition)

[0153] Organic layer **3** (exciton diffusion prevention layer **17**) (20 nm): BCP

[0154] Organic layer **4** (electron transport layer **16**) (40 nm): Alq3

[0155] Metal electrode layer **1** (metal electrode **11**) (15 nm): Al—Li alloy (Li=1.8 wt. %)

[0156] Metal electrode layer **2** (metal electrode **11**) (100 nm): Al

[0157] EL characteristics of the luminescence devices using the metal coordination compounds of formula (1) (Ex. Comp. Nos. 37 and 1) were measured by using a microammeter ("Model 4140B", mfd. by Hewlett-Packard Co.) for a current density under application of a voltage of 20 volts using a luminance meter ("Model BM7", mfd. by Topcon K.K.) for a luminescence efficiency (luminescence luminance). Further, both the above-prepared luminescence devices showed a good rectification characteristic.

[0158] The results are shown below.

Ex. No.	Ex. Comp. No.	Luminance (cd/m^2)
1	37	50
2	1	25

[0159] Each of luminescence states of the organic luminescence devices was similar to that based on photoluminescence (luminescence center wavelength) in the case where each of the luminescence materials (Ex. Comp. Nos. 37 and Ex. Comp. No. 1 as luminescence sources in these examples) was dissolved in toluene.

[0160] Accordingly, luminescence from these organic luminescence devices was found to be resulting from the corresponding luminescence material.

EXAMPLE 3

[0161] A simple matrix-type organic EL device shown in **FIG. 2** was prepared in the following manner.

[0162] On a 1.1 mm-thick glass substrate **21** (75×75 mm), a ca. 100 nm-thick transparent electrode **22** of ITO (as an anode) was formed by sputtering, followed by patterning in a stripe form comprising 100 lines (each having a width of 100 μm and a spacing of 40 μm).

[0163] On the ITO electrode **22**, an organic lamination layer **23** including four organic layers was formed in the same manner as in Example 1.

[0164] Then, on the organic lamination layer **23**, a metal electrode comprising a 10 nm-thick Al—Li alloy layer (Li: 1.3 wt. %) and a 150 nm-thick Al layer (disposed on the Al—Li alloy layer) was formed by vacuum deposition (2.7×10^{-3} Pa (=2×10^{-5} Torr)) with a mask, followed by patterning in a stripe form comprising 100 lines (each having a width of 100 μm and a spacing of 40 μm) arranged to intersect the ITO stripe electrode lines at right angles, thus forming an organic EL device having a matrix of pixels (100×100 pixels).

[0165] The thus-prepared organic EL device was placed in a glove box and driven in a simple matrix manner (frame frequency: 30 Hz,interlace scanning) by applying a driving waveform (drive voltage: 15 to 23 volts, scanning signal voltage: 19 volts, data signal voltage: ±4 volts) as shown in **FIG. 3**.

[0166] As a result, a smooth motion picture display by the organic EL device was confirmed.

EXAMPLE 4

[0167] An organic EL device was prepared in the same manner as in Example 1 except that the metal coordination compound (Ex. Comp. No. 37) was charged to a metal coordination compound of the formula 41 (specifically shown hereinabove).

[0168] When the EL device was supplied with a voltage of 20 volts, stable and high-efficiency yellowish green luminescence resulting from the thienylpyridine ligand of the metal coordination compound of the formula 41 was confirmed. The luminescence was stable even when the EL device was continuously driven for 100 hours.

EXAMPLE 5

[0169] An organic EL device was prepared in the same manner as in Example 1 except that the metal coordination compound (Ex. Comp. No. 37) was charged to a metal coordination compound of the formula 44 (specifically shown hereinabove).

[0170] When the EL device was supplied with a voltage of 20 volts, stable and high-efficiency reddish orange luminescence resulting from the metal coordination compound of the formula 44 was confirmed. The luminescence was stable even when the EL device was continuously driven for 100 hours.

EXAMPLE 6

[0171] An organic EL device was prepared in the same manner as in Example 1 except that the metal coordination compound (Ex. Comp. No. 37) was charged to a metal coordination compound of the formula 46 (specifically shown hereinabove).

[0172] When the EL device was supplied with a voltage of 20 volts, stable and high-efficiency reddish orange luminescence resulting from the metal coordination compound of the formula 46 was confirmed. The luminescence was stable even when the EL device was continuously driven for 100 hours.

EXAMPLE 7

[0173] An organic EL device was prepared in the same manner as in Example 1 except that the metal coordination compound (Ex. Comp. No. 37) was charged to a metal coordination compound of the formula 49 (specifically shown hereinabove).

[0174] When the EL device was supplied with a voltage of 20 volts, stable and high-efficiency reddish orange luminescence resulting from the metal coordination compound of the formula 49 was confirmed. The luminescence was stable even when the EL device was continuously driven for 100 hours.

EXAMPLE 8

[0175] An organic EL device was prepared in the same manner as in Example 1 except that the metal coordination compound (Ex. Comp. No. 37) was charged to a metal coordination compound of the formula 50 (specifically shown hereinabove).

[0176] When the EL device was supplied with a voltage of 20 volts, stable and high-efficiency reddish orange luminescence resulting from the metal coordination compound of the formula 50 was confirmed. The luminescence was stable even when the EL device was continuously driven for 100 hours.

EXAMPLE 9

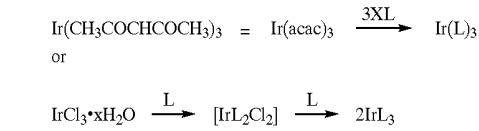
[0177] An organic EL device was prepared in the same manner as in Example 1 except that the metal coordination compound (Ex. Comp. No. 37) was charged to a metal coordination compound of the formula 42 (specifically shown hereinabove).

[0178] When the EL device was supplied with a voltage of 20 volts, stable and high-efficiency green luminescence resulting from the metal coordination compound of the formula 42 was confirmed. The luminescence was stable even when the EL device was continuously driven for 100 hours.

[0179] In the above Examples 4-9, all the metal coordination compounds according to the present invention improved a luminescence efficiency by ca. 20% when compared with corresponding metal coordination compounds having a single luminescent ligand structure, respectively.

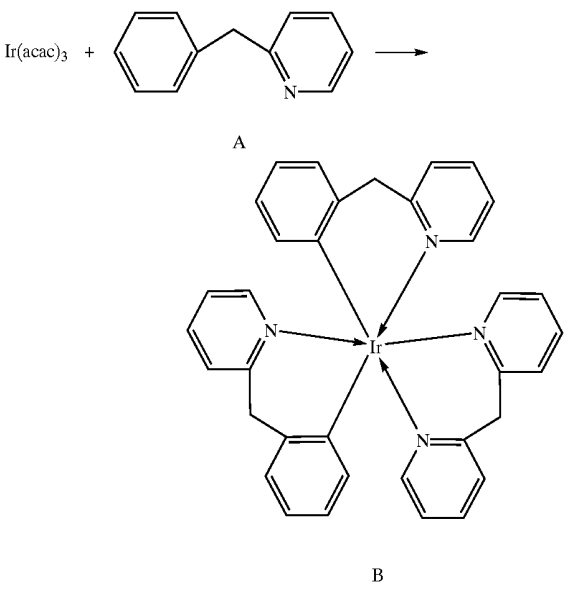
EXAMPLE 10

[0180] Ir-based metal coordination compounds of the formula (1) according to the present invention were basically synthesized through the following reaction schemes.



[0181] In the above, as a starting material, a commercially available Ir acetylacetonato complex or a commercially available hydrated Ir chloride was used. "L" denotes a ligand of an objective Ir complex.

[0182] In a specific synthesis example, a metal coordination compound (Ex. Comp. No. 49) was prepared in the following manner.



[0183] In a 100-four-necked flask, 50 ml of glycerol was placed and stirred for 2 hours at 130-140° C. while supplying nitrogen gas into glycerol, followed by cooling by standing to 100° C. At that temperature, 1.02 g (5.0 mM) of 2-benzylpyridine of formula A and 0.5 g (1.0 mM) of Ir(III) acetyl-acetonate ($Ir(acac)_3$) were added to the system, followed by stirring for 7 hours at ca. 210° C. in a nitrogen gas stream atmosphere.

[0184] The reaction mixture was cooled to room temperature and poured into 300 ml of 1N-hydrochloric acid. The resultant precipitate was recovered by filtration and washed with water, followed by purification by silica gel column chromatography (eluent: chloroform) to obtain 0.11 g of a black solid metal coordination compound (Ex. Comp. No. 49 of formula B) (Yield: 16%).

[0185] The thus-prepared metal coordination compound was subjected to MALDI-TOF-MS (Matrix-assisted Laser Desorption Ionization mass spectroscopy), whereby M^+ (mass number of ionized objective product) of 697.2 (as a molecular weight) was confirmed.

[0186] When the metal coordination compound was dissolved in toluene and subjected to measurement of luminescence spectrum, the metal coordination compound provided a luminescence spectrum diagram including a maximum luminescence wavelength λmax of 463 nm as shown in **FIG. 5**.

[0187] Further, when $Ir(ppy)_3$ described hereinabove was used as a standard compound exhibiting a phosphorescence yield φ ($Ir(ppy)_3$) of 1, the metal coordination compound (Ex. Comp. No. 49) exhibited a phosphorescence yield φ (unknown) of 0.6.

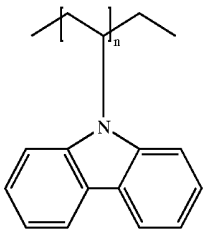
[0188] Herein, the phosphorescence yield φ (φ (unknown)) may be obtained according to the following equation:

$$\phi\ (\text{unknown})/\phi\ (Ir(ppy)_3) = [Sem\ (\text{unknown})/Iabs\ (\text{unknown})]/[Sem\ (Ir(ppy)_3)/Iabs\ (Ir(ppy)_3)],$$

[0189] wherein φ (unknown) represents a phosphorescence yield of an unknown (objective) compound, φ ($Ir(ppy)_3$) represents a phosphorescence yield of $Ir(ppy)_3$ (=1 in this case) Sem (unknown) represents an absorption coefficient of an unknown compound at its excitation wavelength, Iabs (unknown) represents an areal intensity of emission spectrum of the unknown compound excited at the excitation wavelength, Sem ($Ir(ppy)_3$ represents an absorption coefficient of $Ir(ppy)_3$ at its excitation wavelength, and Iabs ($Ir(ppy)_3$) represents an areal intensity of emission spectrum of $Ir(ppy)_3$ excited at the excitation wavelength.

EXAMPLE 11

[0190] In this example, the metal coordination compound (Ex. Comp. No. 49) prepared in Example 10 was mixed with polyvinyl carbazole (PVK) shown below in a weight ratio of 8:92 to obtain a luminescent material used for a luminescence layer.



[0191] An organic EL device was prepared in the following manner.

[0192] A 1.1 mm-thick glass substrate provided with a 70 nm-thick ITO electrode (as an anode electrode) was subjected to plasma-ozone washing.

[0193] On the thus-treated glass substrate, a solution of the above-prepared luminescent material (mixture of the metal coordination compound (Ex. Comp. No. 49) and PVK) in chloroform was spin-coated at 2000 ppm, followed by drying to obtain a luminescence layer having a thickness of 90±10 nm.

[0194] The thus-treated glass substrate was then placed in a vacuum deposition chamber. On the luminescence layer of the substrate, a 30 nm-thick Mg—Ag alloy layer and a 100 nm-thick Al layer (as a cathode electrode) were successively

formed by vacuum deposition (at most 10-4 Pa), thus preparing an organic EL device.

[0195] When a DC voltage of 8-12 volts was applied between the ITO electrode (anode) and the metal electrode (cathode), clear blue luminescence was confirmed.

[0196] Further, the luminescence material (mixture) after drying exhibited a maximum luminescence wavelength was 490 nm closer to that (473 nm) of the metal coordination compound (Ex. Comp. No. 49) in toluene solution used in Example 10. Accordingly, the luminescence in this example was resulting from the metal coordination compound (Ex. Comp. No. 49).

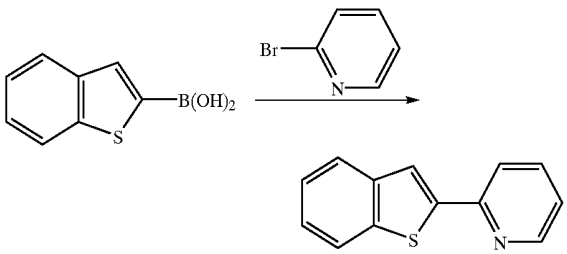
[0197] After the DC voltage application, an attenuation time for the blue luminescence was at least 0.3-0.5 sec. As a result, the blue luminescence in this example was supported to be phosphorescence attributable to the metal coordination compound (Ex. Comp. No. 49).

[0198] The blue luminescence state was stable even when the EL device was continuously driven for 12 hours.

EXAMPLES 12 AND 13

[0199] In these examples, metal coordination compound (of formulas 43 and 51 specifically shown above) were synthesized through the following steps 1) to 4).

[0200] Step 1) (Synthesis of 2-(pyridine-2-yl)benzo[b]-thiophene

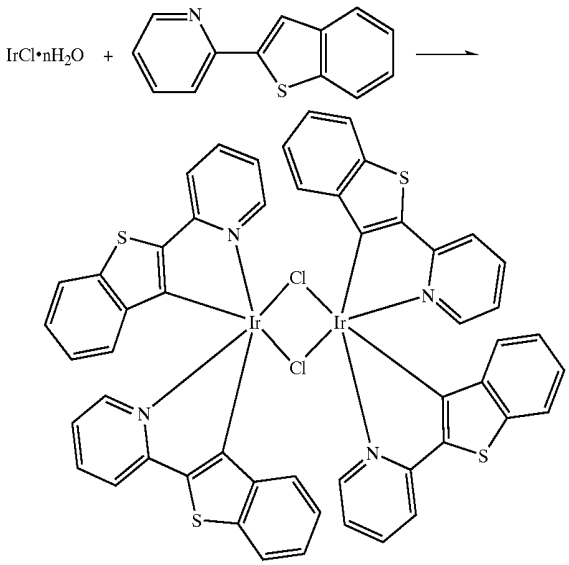


[0201] In a 1 liter-three-necked flask, 26.6 g (168.5 mM) of 2-bromopridine, 30.0 g (168.5 mM) of benzo[b] thiophene-2-boric acid, 170 ml of toluene, 85 ml of ethanol and 170 ml of 2M-sodium carbonate aqueous solution were placed, and to the mixture, under stirring in a nitrogen gas stream atmosphere, 6.18 g (5.35 mM)of tetrakis-(triphenylphosphin) palladium (O) was added, followed by refluxing under stirring for 5.5 hours in a nitrogen gas stream atmosphere.

[0202] After the reaction, the reaction mixture was cooled and subjected to extraction with cold water and toluene.

[0203] The organic layer was washed with water until the layer became neutral, followed by distilling-off of the solvent under reduced pressure to obtain a residue. The residue was purified by silica gel column chromatography (eluent: toluene/hexane=5/1) and then by alumina column chromatography (eluent: toluene) and was recrystallized from ethanol to obtain 12.6 g o 2-(pyridine-2-yl)benzo[b]thiophene (Yield: 35.4%).

[0204] Step 2) (Synthesis of tetrakis(2-benzo[b]-thiophene-2-yl)pyridine-C^3,N)(μ-dichloro)diiridium (III)

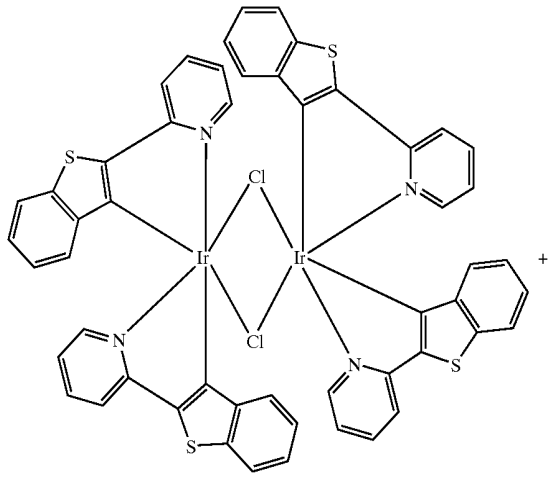


[0205] In a 500 ml-three-necked flask, 3.65 g (10.4 mM) of n-hydrated iridium (III) chloride ($IrCl \cdot nH_2O$), 4.82 g (22.8 mM) of 2-(benzo[b]thiophene-2-yl)pyridine, 150 ml of 2-ethoxy ethanol and 50 ml of water were placed and stirred for 0.5 hour at room temperature in an argon gas atmosphere. The mixture was then gradually heated and subjected to refluxing for ca. 24 hours under stirring.

[0206] After cooling, the reaction mixture was subjected to filtration, followed by washing with ethanol and acetone.

[0207] The resultant powder was dissolved in chloroform and subjected to extraction with water. The organic layer was dried with anhydrous magnesium sulfate, followed distilling-off of the solvent to obtain a residue. The residue was recrystallized from a mixture solvent (hexanemethylene chloride) to obtain 5.40 g of tetrakis(2-(benzo[b]thiophene-2-yl)pyridine-C^3, N) (μ-dichloro)diiridium (III) (Yield: 80.1%).

[0208] Step 3) Synthesis of bis(2-(benzo[b]thiophene-2-yl)pyridine-C^3,N) (acetylacetonato)iridium (III)



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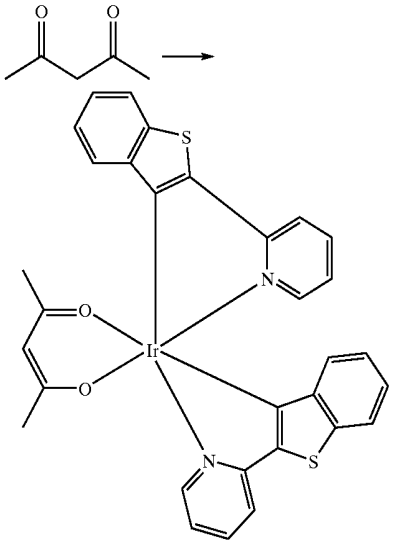
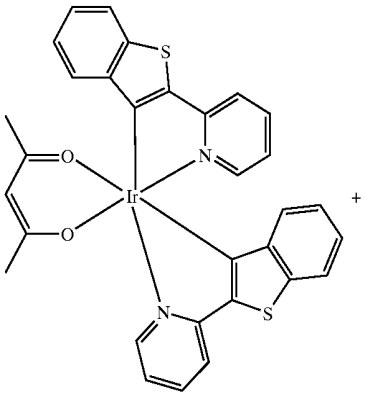


[0209] In a 500 ml-three-necked flask, 2.2 g (1.70 mM) of tetrakis (2-(benzo[b]thiophene-2-yl) pyridine-C^3,N) (μ-dichloro)diiridium, 0.51 g (5.09 mM) of acetylacetone, 2.5 g of sodium carbonate and 150 ml of ethanol were placed and stirred for 1 hour in an argon gas stream atmosphere.

[0210] The mixture was then gradually heated and subjected to refluxing for 15 hours under stirring.

[0211] After the reaction, the reaction mixture was cooled. The resultant precipitate was recovered by filtration and washed with water and ethanol to obtain a residue. The residue was purified by silica gel column chromatography (eluent: chloroform) and recrystallized from ethanol to obtain 1.87 g of bis(2-(benzo[b]thiophene-2-yl)pyridine-C^3,N) (acetylacetonato)iridium (III) (Yield: 77.3%).

[0212] Step 4) (Synthesis of bis(2-(benzo[b]thiophene-2-yl)pyridine-C^3,N) (phenylpyridine-C^2,N) iridium (III) (metal coordination compound of formula 51) and bis(phenylpyridine-C^2,N) (2-(benzo[b]thiophene-2-yl)pyridine-C^3, N) iridium (III) (metal coordination compound of formula 43))



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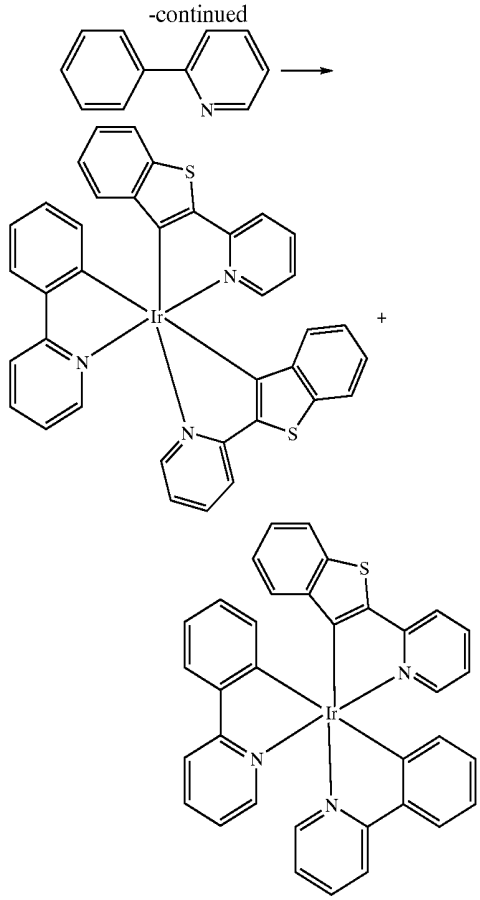


[0213] In a 100 ml-three-necked flask, 50 ml of glycerol was placed and air in the interior of the flask was aerated with argon gas. Under stirring, 0.7 g (1.00 mM) of bis(2-benzo[b]thiophene-2-yl) pyridine-C^3,N) (acetylacetonato)iridium (III) and 0.39 g (2.50 mM) of 2-phenylpyridine were added to the glycerol, followed by stirring for 10 hours at 200° C.

[0214] After the reaction, to the reaction mixture, 300 ml of 1N-hydrochloric acid was added, followed by filtration. The resultant residue was purified by silica gel column chromatography (eluent: chloroform) and then fractionation by high-performance liquid chromatography to obtain 108 mg of bis(2-(benzo[b]thiophene-2-yl)pyridine-C^3,N) (phenylpyridine-C^2,N)iridium (III) (metal coordination compound of formula 51) and 35 mg of bis(phenylpyridine-C^2, N) (2-(benzo[b]thiophene-2-yl)pyridine-C^3,N) iridium (III) (metal coordination compound of formula 43)).

[0215] The thus-prepared metal coordination compounds (of formulas 51 and 43) were subjected to MALDI-TOF-MS, respectively, whereby $M^+$of 767.1 for the metal coordination compound of formula 51 and M^+ of 711.1 for the metal coordination compound of formula 43 were confirmed, respectively.

[0216] When each of the metal coordination compounds of formulas 51 and 43 was dissolved in toluene and are subjected to measurement of luminescence spectrum, both the metal coordination compounds of formulas 51 and 43 exhibited a maximum luminescence wavelength λmax of

598 nm, thus confirming that the luminescence was attributable to the benzothienyl ligand.

[0217] Further, when $Ir(ppy)_3$ described hereinabove was used as a standard compound exhibiting a phosphorescence yield ϕ of 1, the metal coordination compound of formula 51 exhibited a phosphorescence yield ϕ of 0.2 and the metal coordination compound of formula 43 exhibited a phosphorescence yield ϕ of 0.3.

[0218] In order to confirm that the luminescence was phosphorescence, each of the metal coordination compounds of formulas 51 and 43 was dissolved in chloroform to prepare a first solution and a second solution. Each first solution was subjected to aeration with oxygen gas and each second solution was subjected to aeration with nitrogen gas.

[0219] When each of the thus-prepared first and second solutions were subjected to light irradiation, the oxygen-aerated solution exhibited substantially no phosphorescence but the nitrogen-aerated solution exhibited phosphorescence. As a result, these metal coordination compounds of formulas 51 and 43 were found to be phosphorescent metal coordination compounds.

[0220] The metal coordination compounds of formulas 51 and 43 were then subjected to measurement of luminescence life (time) in the following manner. by Each of the metal coordination compounds of formulas 51 and 43 was dissolved in chloroform and was spin-coated on a quartz substrate to form a ca. 0.1 μm-thick metal coordination compound layer.

[0221] By using a luminescence life-measuring apparatus (available from Hamamatsu Photonics K.K.), the above-prepared metal coordination compound layer formed on the substrate was subjected to pulse irradiation with nitrogen laser light (excitation wavelength: 337 nm) at room temperature to measure an attenuation time immediately after the excitation laser pulse irradiation.

[0222] A luminescence intensity I after a lapse of t (sec) is defined as the following equation:

$$I=I_0\exp(-t/\tau),$$

[0223] wherein I_0 represents an initial luminescence intensity and τ (μsec) represents a luminescence life (time).

[0224] As a result, both the metal coordination compounds of formulas 51 and 43 showed a shorter luminescence life of at most 10 μsec.

[0225] Accordingly, the metal coordination compound of the present invention is expected to provide an organic EL device sing the metal coordination compound with a good stability since the metal coordination compound exhibits phosphorescent luminescence and a shorter phosphorescence life (time).

EXAMPLES 14 AND 15

[0226] Two organic EL devices using the metal coordination compound of formulas 51 and 43 prepared in Examples 12 and 13 were prepared in these examples.

[0227] Each of the organic luminescence devices had a structure including four organic (compound) layers (luminescence function layers) shown in **FIG. 1**C and was prepared in the following manner.

[0228] On a 1.1 mm-thick glass substrate (transparent substrate **15**), a 100 nm-thick film (transparent electrode **14**) of ITO (indium tin oxide) was formed by sputtering, followed by patterning to have an (opposing) electrode area of 3 mm^2.

[0229] On the ITO-formed substrate, four organic layers and two metal electrode layers shown below were successively formed by vacuum (vapor) deposition using resistance heating in a vacuum chamber (10^{-4} Pa).

[0230] Organic layer **1** (hole transport layer **13**) (50 nm): α-NPD

[0231] Organic layer **2** (luminescence layer **12**) (40 nm): CBP: metal coordination compound of formula (1) (93:7 by weight) (co-vacuum deposition)

[0232] Organic layer **3** (exciton diffusion prevention layer **17**) (20 nm): BCP

[0233] Organic layer **4** (electron transport layer **16**) (40 nm): Alq3

[0234] Metal electrode layer **1** (metal electrode **11**) (15 nm): Al—Li alloy (Li=1.8 wt. %)

[0235] Metal electrode layer **2** (metal electrode **11**) (100 nm): Al

[0236] EL characteristics of the luminescence devices using the metal coordination compounds of formulas 51 and 43 were measured by using a microammeter ("Model 4140B", mfd. by Hewlett-Packard Co.) for a current density under application of a voltage of 8 volts (current-voltage characteristic), using a spectrophotofluoro-meter ("Model SR1", mfd. by Topcon K.K.) for a maximum luminescence wavelength λmax, and using a luminance meter ("Model BM7", mfd. by Topcon K.K.) for a luminescence efficiency. Further, both the above-prepared luminescence devices showed a good rectification characteristic.

[0237] The results are shown below.

Ex. No.	Formula	λmax (nm)	Luminance (cd/m^2)
14	51	598	1.0
15	43	597	2.1

[0238] Each of luminescence states of the organic EL devices was similar to that based on photoluminescence in the case where each of the luminescence materials was dissolved in toluene.

[0239] Accordingly, luminescence from these organic EL devices was found to be resulting from the respective metal coordination compounds of formulas 51 and 43.

[0240] Further, as apparent from the above results, the metal coordination compound of formula 43 effectively improved the luminescence efficiency when compared with the metal coordination compound of formula 51.

[0241] In these metal coordination compounds of formulas 43 and 51, the luminescent ligand was the benzothienylpyridine ligand and thus the luminescence efficiency was found to be dependent upon the number of the benzothienylpyridine ligand.

[0242] According to these examples (Examples 14 and 15), it was confirmed that a lesser number of the benzothienylpyridine ligand (constituting the metal coordination compound of formula 43) as the luminescent ligand was more effective in improving the luminescence efficiency.

[0243] As described hereinabove, according to the present invention, it is possible to provide a metal coordination compound of the formula (1) suitable as a luminescent material for broader wavelength range luminescence of an organic EL device and exhibiting a higher phosphorescence yield and a shorter phosphorescence life (time). An organic luminescence device (EL device) using the metal coordination compound according to the present invention stably exhibits high-efficiency luminescence.

What is claimed is:

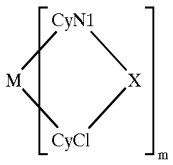
1. A metal coordination compound represented by the following formula (1):

$$LmML'n \quad (1),$$

wherein M denotes Ir, Pt, Ph or Pd; L denotes a bidentate ligand; L' denotes a bidentate ligand different from L; m is an integer of 1, 2 or 3; and n is an integer of 0, 1 or 2 with the proviso that the sum of m and n is 2 or 3,

the partial structure MLm being represented by a formula (2) or a formula (3) shown below, and the partial structure ML'n being represented by a formula (4) or a formula (5) shown below:

(2)



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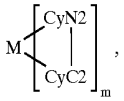

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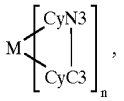

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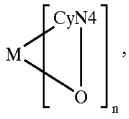


wherein CyN1, CyN2 and CyN3 independently denote a substituted or unsubstituted cyclic group containing a nitrogen atom connected to M; CyN4 denotes a cyclic group containing 8-quinoline or its derivative having a nitrogen atom connected to M; CyC1, CyC2 and CyC3 independently denote a substituted or unsubstituted cyclic group containing a carbon atom connected to M,

each of substituents for CyN1, CyN2, CyN3, CyC1, CyC2 and CyC3 being selected from the group consisting of a halogen atom; cyano group; nitro group; a trialkylsilyl group containing three linear or branched alkyl groups each independently having 1-8 carbon atoms; a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom; and an aromatic ring group capable of having a substituent selected from the group consisting of a halogen atom; cyano group; nitro group; and a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom,

CyN1 and CyC1 being connected via a covalent group containing X which is represented by —O—, —S—, —CO—, —C(R1)(R2)— or —NR— where R1, R2 and R independently denote a hydrogen atom, a halogen atom, an alkyl group, an alkyl group substituted with a halogen atom, a phenyl group or a naphthyl group, and

CyN2 and CyC2, and CyN3 and CyC3 being independently connected via a covalent bond,

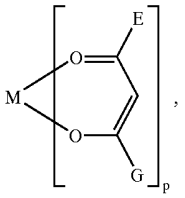
with the proviso that the metal coordination compound is represented by the formula (2) when n is 0.

2. A compound according to claim 1, wherein the partial structure MLm is represented by the formula (2).

3. A compound according to claim 2, wherein M is Ir.

4. A compound according to claim 2, wherein the metal coordination compound has another partial structure represented by the following formula (6):

(6)



wherein M denotes Ir, Pt, Ph or Pd; p is 1; and E and G independently denote a linear or branched alkyl group having 1-20 carbon atom capable of including a hydrogen atom which can be replaced with a fluorine atom, or an aromatic ring group capable of having a substituent selected from the group consisting of a halogen atom; cyano group; nitro group; a trialkylsilyl group containing three linear or branched alkyl groups each independently having 1-8 carbon atoms; and a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom.

5. A compound according to claim 1, which exhibits a phosphorescence at the time of energy transition from an excited state to a ground state.

6. A compound according to claim 1, wherein one of the ligands L and L' is a luminescent ligand and the other ligand is a carrier transport ligand.

7. A compound according to claim 1, wherein at least one of the ligands L and L' is in a metal to ligand charge transfer excited state.

8. A compound according to claim 1, wherein the ligands L and L' includes a first ligand capable of providing a first maximum luminescence wavelength λ1 based on an excited state thereof and a second ligand capable of providing a second maximum luminescence wavelength λ2 shorter than λ1, the number of the first ligand providing λ1 being smaller than that of the second ligand providing λ2.

9. A compound according to claim 1, wherein the ligands L and L' includes a stronger luminescent ligand and a weaker luminescent ligand, the number of the stronger luminescent ligand is smaller than that of the weaker luminescent ligand.

10. An organic luminescence device, comprising: a substrate, a pair of electrodes disposed on the substrate, and a luminescence function layer disposed between the pair of electrodes comprising at least one species of an organic compound,

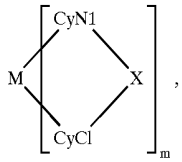
wherein the organic compound comprises a metal coordination compound represented by the following formula (1):

LmML'n (1),

wherein M denotes Ir, Pt, Ph or Pd; L denotes a bidentate ligand; L' denotes a bidentate ligand different from L; m is an integer of 1, 2 or 3; and n is an integer of 0, 1 or 2 with the proviso that the sum of m and n is 2 or 3,

the partial structure MLm being represented by a formula (2) or a formula (3) shown below, and the partial structure ML'n being represented by a formula (4) or a formula (5) shown below:

(2)



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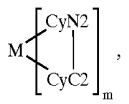

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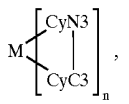

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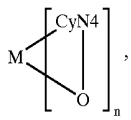

wherein CyN1, CyN2 and CyN3 independently denote a substituted or unsubstituted cyclic group containing a nitrogen atom connected to M; CyN4 denotes a cyclic group containing 8-quinoline or its derivative having a nitrogen atom connected to M; CyC1, CyC2 and CyC3 independently denote a substituted or unsubstituted cyclic group containing a carbon atom connected to M,

each of substituents for CyN1, CyN2, CyN3, CyC1, CyC2 and CyC3 being selected from the group consisting of a halogen atom; cyano group; nitro group; a trialkylsilyl group containing three linear or branched alkyl groups each independently having 1-8 carbon atoms; a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom; and an aromatic ring group capable of having a substituent selected from the group consisting of a halogen atom; cyano group; nitro group; and a linear or branched alkyl group having 1-20 carbon atoms capable of including one or at least two non-neighboring methylene groups which can be replaced with —O—, —S—, —CO—, —CO—O—, —O—CO—, —CH═CH— or —C≡C— and capable of including a hydrogen atom which can be replaced with a fluorine atom,

CyN1 and CyC1 being connected via a covalent group containing X which is represented by —O—, —S—, —CO—, —C(R1)(R2)— or —NR— where R1, R2 and R independently denote a hydrogen atom, a halogen atom, an alkyl group, an alkyl group substituted with a halogen atom, a phenyl group or a naphthyl group, and

CyN2 and CyC2, and CyN3 and CyC3 being independently connected via a covalent bond,

with the proviso that the metal coordination compound is represented by the formula (2) when n is 0.

11. A device according to claim 10, wherein the partial structure MLm is represented by the formula (2).

12. A device according to claim 11, wherein M is Ir.

13. A device according to claim 10, wherein a voltage is applied between the pair of electrodes to cause phosphorescence from the luminescence function layer.

14. An image display device, comprising: an organic luminescence device according to claim 10 and means for supplying electrical signals to the organic luminescence device.

* * * * *

专利名称(译)	金属配位化合物，发光装置和显示装置		
公开(公告)号	US20030054198A1	公开(公告)日	2003-03-20
申请号	US09/995608	申请日	2001-11-29
[标]申请(专利权)人(译)	坪山AKIRA MIZUTANI秀昌 冈田治郎 泷口TAKAO 三浦诚志 野口KOJI MORIYAMA TAKASHI 井川聪 镰谷JUN FURUGORI MANABU		
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IPC分类号	H01L51/50 C07D213/06 C07D213/50 C07D213/64 C07D215/24 C07D409/04 C07F15/00 C09K11/06 H01L51/00 H01L51/30 H05B33/14		

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其他公开文献	US6991857
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摘要(译)

一种有机EL器件，包括发光层，所述发光层含有长时间高发光和高效发光的发光材料，由下式（1）表示的金属配位化合物：LmML'n，其中M表示Ir，Pt，Ph或Pd; L表示二齿配体; L'表示与L不同的二齿配体; m是1,2或3的整数; n是0,1或2的整数，条件是m和n之和为2或3.部分结构MLm由下面的公式（2）或公式（3）表示，部分结构结构ML'n由下面所示的式（4）或式（5）表示：其中CyN1，CyN2和CyN3独立地表示含有与M连接的氮原子的取代或未取代的环状基团; CyN4表示含有8-喹啉或其衍生物的环状基团，其具有与M连接的氮原子; CyC1，CyC2和CyC3独立地表示含有与M连接的碳原子的取代或未取代的环状基团，条件是当n为0时，金属配位化合物由式（2）表示。