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(54) POLYCYCLIC COMPOUNDS AND ORGANIC ELECTROLUMINESCENCE DEVICE EMPLOYING THE SAME

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(57) ABSTRACT

Provided are a polycyclic compound of a compound having such a structure that two benzene rings bond to a central benzene ring each other to form a fused ring and another fused ring bonds to a terminal thereof, and an organic electroluminescence device including one or more organic thin film layers containing a light emitting layer between a cathode and an anode, in which at least one of the organic thin film layers includes the polycyclic compound of the present invention. The organic electroluminescence device has high luminous efficiency, no defect in pixels, and long lifetime. In addition, provided is a polycyclic compound realizing the organic electroluminescence device.

24 Claims, No Drawings

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POLYCYCLIC COMPOUNDS AND ORGANIC ELECTROLUMINESCENCE DEVICE EMPLOYING THE SAME

This is a continuation application of U.S. application Ser. ⁵ No. 12/414,050, filed Mar. 30, 2009.

TECHNICAL FIELD

The present invention relates to a polycyclic compound ¹⁰ and an organic electroluminescence device using the polycyclic compound, in particular, an organic electroluminescence device, which shows high luminous efficiency and has a long lifetime, and a polycyclic compound for realizing the device.

BACKGROUND ART

An organic electroluminescence device (hereinafter, "electroluminescence" may be abbreviated as "EL") is a spontaneous light emitting device which utilizes the principle that a 20 fluorescent substance emits light by energy of recombination of holes injected from an anode and electrons injected from a cathode when an electric field is applied. Since a laminate type organic EL device driven under a low electric voltage was reported, many studies have been conducted on organic 25 EL devices using organic materials as the constituent materials. The devices of the laminate type use tris(8-quinolinolato) aluminum for a light emitting layer and a triphenyldiamine derivative for a hole transporting layer. Advantages of the laminate structure are that the efficiency of hole injec- 30 tion into the light emitting layer can be increased, that the efficiency of forming exciton which are formed by blocking and recombining electrons injected from the cathode can be increased, and that exciton formed within the light emitting layer can be enclosed. As described above, for the structure of 35 the organic EL device, a two-layered structure having a hole transporting (injecting) layer and an electron transporting light emitting layer and a three-layered structure having a hole transporting (injecting) layer, a light emitting layer, and an electron transporting (injecting) layer are well known. To 40 increase the efficiency of recombination of injected holes and electrons in the devices of the laminate type, the structure of the device and the process for forming the device have been studied.

As the light emitting material of the organic EL device, 45 chelate complexes such as tris(8-quinolinolato) aluminum complexes, light emitting materials such as coumarin derivatives, tetraphenylbutadiene derivatives, distyrylarylene derivatives, and oxadiazole derivatives are known. It is reported that light in the visible region ranging from blue light to red light can be obtained by using these light emitting materials, and realization of a device exhibiting color images is expected.

Patent Doc Non-patent No. 3, pp 442 Non-patent 50 No. 1, pp 4-6 DIS

In addition, it has been recently proposed that a phosphorescent material as well as a fluorescent material be utilized in 55 the light emitting layer of an organic EL device. High luminous efficiency is achieved by utilizing the singlet and triplet states of an excited state of an organic phosphorescent material in the light emitting layer of an organic EL device. Upon recombination of an electron and a hole in an organic EL device, singlet excitons and triplet excitons may be produced at a ratio of 1:3 owing to a difference in spin multiplicity between the singlet and triplet excitons, so the use of a phosphorescent material may achieve luminous efficiency three to four times as high as that of a device using fluorescence alone.

Patent Documents 1 to 4 are exemplary inventions each describing such materials for an organic EL device.

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Patent Document 1 describes a compound using, as a mother skeleton, a structure obtained by crosslinking a terphenylene skeleton with, for example, a carbon atom, nitrogen atom, or oxygen atom. The document, which mainly discloses data indicative of the potential of the compound to serve as a hole transporting material, describes that the compound is used as a host material for a phosphorescent material in a light emitting layer. However, the description is limited to a red phosphorescent device, and the luminous efficiency of the device is not high enough for practical use.

Patent Document 2 describes an indolocarbazole compound having a substituent on a nitrogen atom or on an aromatic ring. The document recommends that the compound be used as a hole transporting material, and describes that a thermally and morphologically stable, thin hole transporting layer can be prepared from the compound. However, the document does not describe data indicative of the usefulness of the compound as a host material or electron transporting material to be used together with a phosphorescent material.

Patent Document 3 describes indolocarbazole compounds each having a substituent on a nitrogen atom or on an aromatic ring. The document discloses data on a green light emitting device using any one of those compounds as a host material for a phosphorescent material in its light emitting layer. However, a high voltage must be applied to the device to drive the device, and the device shows low luminous efficiency, so the device cannot be sufficiently put into practical use.

Patent Document 4 describes indolocarbazole compounds each having a substituent. The document describes that each of the compounds functions as a host material for a phosphorescent material in a light emitting layer. However, each of those compounds is characterized in that the compound has a dimer or trimer structure through a linking group, and each of the compounds tends to have a large molecular weight. The document discloses data on a green phosphorescent device using any one of those compounds, but all the compounds used each have a large molecular weight of 800 or more. The efficiency with which a material having a large molecular weight is deposited in a vacuum is poor, and the material may decompose owing to heating for a long time period, so the material may be insufficient in terms of practical use.

Patent Document 1: WO 2006/122630

Patent Document 2: EP 0908787

Patent Document 3: WO 2007/063796

Patent Document 4: WO 2007/063754

Non-patent Document 1: Applied Physics letters Vol. 74 No. 3, pp 442-444

Non-patent Document 2: Applied Physics letters Vol. 75 No. 1, pp 4-6

DISCLOSURE OF THE INVENTION

Problems to be Solved by the Invention

The present invention has been made with a view to solving the above problems, and an object of the present invention is to provide an organic EL device which shows high luminous efficiency and has a long lifetime, and a polycyclic compound for realizing the device.

Means for Solving the Problems

The inventors of the present invention have extensively studied in order to achieve the above object. As a result, the inventors found that the above object could be achieved by using, as a material for an organic EL device, a polycyclic

(1)

(3a)

(3b)

3

compound represented by the following formula (1) or (2) and having such a structure that two benzene rings bonds to the ortho, meta, or para position of the central benzene ring to form a fused ring, and another fused ring represented by the following general formula (4) bonds to the terminal thereof, ⁵ thereby completing the present invention.

That is, the present invention provides a polycyclic compound represented by the following formulae (1) or (2):

[Chem 1] $\begin{bmatrix} L_1 J_o & & & & \\ & Y_1 & & & & \\ & & & X_1 & & & \\ & & & & & X_1 & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ &$

[In the general formulae (1) and (2), a ring A represents a benzene ring represented by the above formula (3a) which is $_{45}$ fused to two adjacent rings at arbitrary positions and a structure B represents a structure represented by the above formula (3b) which is fused to the ring A to share a ring-forming carbons C_1 and C_2 .

In the general formulae (1) and (2), X_1 and X_2 each inde- 50 pendently represent oxygen (O), sulfur (S), N-R₁, or CR₂R₃, and R₁, R₂, and R₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsub- 55 stituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic het- 60 erocyclic group having 3 to 24 atoms forming the aromatic ring, provided that when both X_1 and X_2 represent N— R_1 , at least one R₁ represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring.

In the general formulae (1) and (2), o, p, q, and r each independently represent 0 or 1, provided that o+p is 1 or more.

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In the general formula (2), n represents 2, 3, or 4.

In the general formulae (1) and (2), L_1 , L_2 , L_{3a} , and L_{3b} each independently represent a structure represented by the general formula (4), Ar₁ and Ar₂ each independently represent a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, E represents a single bond, oxygen (O), sulfur (S), 10 N—R₄, or CR₅R₆, and R₄, R₅, and R₆ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon 15 atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the 20 aromatic ring.

In the general formula (2), when n represents 2, L₄ represents a single bond, oxygen (O), sulfur (S), CO, SO, PO, SO₂, —R₇, a substituted or unsubstituted alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted 25 cycloalkylene group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, R7 represents a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, when n represents 3, L₄ represents N, a substituted or unsubstituted alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetrivl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom. a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, and when n represents 4, L4 represents a substituted or unsubstituted alkane tetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formula (1) or (2), Y_1 , Y_2 , and Y_3 each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, or a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having

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6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring which is bonded with a carbon atom, the number of Y_1 's is 0, 1, 2, or 3, the number of Y_2 's is 0, 1, 2, 3, or 4, and the number of Y_3 's is 0, 1, or 2;

provided that: there is no case where the general formula (1) has a structure represented by the following general formula (5):

where R_2 , R_3 , L_1 , L_2 , L_3 , Y_1 , Y_2 , Y_3 , o, p, and q each have the same meanings as R_2 , R_3 , L_1 , L_2 , L_{3a} , Y_1 , Y_2 , Y_3 , o, p, and q in the formula (1); and

there is no case where the general formula (2) has a structure represented by the following general formula (6):

[Chem 3] 30 (6)

$$\begin{bmatrix} [L_1]_o & & & \\ Y_1 & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$$

where R_2 , R_3 , L_1 , L_2 , L_3 , L_4 , Y_1 , Y_2 , Y_3 , o, p, q, and n each have the same meanings as R_2 , R_3 , L_1 , L_2 , L_{3a} , L_4 , Y_1 , Y_2 , Y_3 , a, p, q, and n in the formula (2).]

In addition, the present invention provides an organic EL device having one or more organic thin film layers including a light emitting layer between a cathode and an anode in which at least one layer of the organic thin film layers contains the polycyclic compound.

Further, the polycyclic compound can be used also as an organic solar cell, organic semiconductor laser, a sensor using organic matter, or a material for an organic electron device used in an organic TFT.

Effects of the Invention

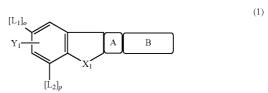
According to the present invention, there can be provided an organic EL device which shows high luminous efficiency and has a long lifetime, and a polycyclic compound for realizing the device.

BEST MODE FOR CARRYING OUT THE INVENTION

The polycyclic compound of the present invention is represented by the following formula (1) or (2):

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[Chem 4]



$$\begin{bmatrix} [L_1]_o \\ Y_1 \end{bmatrix} \underbrace{ \begin{bmatrix} [L_2]_p \end{bmatrix}}_{X_1} A \underbrace{ B} \underbrace{ \begin{bmatrix} [L_2]_p \end{bmatrix}}_{X_1} \underbrace{ \begin{bmatrix} [L_2]_o \end{bmatrix}}_$$

$$-N$$

$$Ar_1$$

$$Ar_2$$

$$Ar_2$$

In the general formulae (1) and (2), a ring A represents a benzene ring represented by the above formula (3a) which is fused to two adjacent rings at arbitrary positions and a structure B represents a structure represented by the above formula (3b) which is fused to the ring A to share a ring-forming 40 carbons C_1 and C_2 .

In the general formulae (1) and (2), X_1 and X_2 each independently represent oxygen (O), sulfur (S), N-R₁, or CR₂R₃, and R₁, R₂, and R₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, provided that when both X_1 and X_2 represent $N-R_1$, at least one R₁ represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring.

In the general formulae (1) and (2), o, p, q, and r each independently represent 0 or 1, provided that o+p is 1 or more. In addition, the case where q+r is 1 or less is preferred from the viewpoint of practical use, because the molecular weight of the polycyclic compound becomes small, the efficiency of the vacuum vapor deposition is improved, and decomposition due to long-time heating is suppressed.

In the general formula (2), n represents 2, 3, or 4.

In the general formulae (1) and (2), L_1 , L_2 , L_{3a} , and L_{3b} each independently represent a structure represented by the general formula (4), Ar_1 and Ar_2 each independently repre-

sent a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, E represents a single bond, oxygen (O), sulfur (S), 5 N—R₄, or CR₅R₆, and R₄, R₅, and R₆ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon 10 atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the 15 aromatic ring

In the general formula (2), when n represents 2, L₄ represents a single bond, oxygen (O), sulfur (S), CO, SO, PO, SO₂, N—R₇, a substituted or unsubstituted alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted 20 cycloalkylene group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aro- 25 matic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, R₇ represents a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the 30 ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsub- 35 stituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, further, when n represents 3, L₄ represents N, a substituted or unsubstituted alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming 40 the ring, a substituted or unsubstituted trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aro- 45 matic heterocyclic group having 3 to 24 atoms forming the aromatic ring, and when n represents 4, L4 represents a substituted or unsubstituted alkane tetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, a 50 silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formula (1) or (2), Y₁, Y₂, and Y₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, or a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted or unsubstituted or unsubstituted or unsubstituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, which is bonded with

a carbon atom, the number of Y_1 's is 0, 1, 2, or 3, the number of Y_2 's is 0, 1, 2, 3, or 4, and the number of Y_3 's is 0, 1, or 2;

provided that: there is no case where the general formula (1) has a structure represented by the following general formula (5):

[Chem 5]

$$\begin{array}{c} R_2 & R_3 \\ Y_1 & & & \\ IL_2|_p & & & \\ R_2 & R_3 & & \\ Y_3 & & & \\ Y_2 & & & \\ \end{array}$$

where R_2 , R_3 , L_1 , L_2 , L_3 , Y_1 , Y_2 , Y_3 , o, p, and q each have the same meanings as R_2 , R_3 , L_1 , L_2 , L_{3a} , Y_1 , Y_2 , Y_3 , o, p, and q in the formula (1); and

there is no case where the general formula (2) has a structure represented by the following general formula (6):

[Chem 6]

$$\begin{bmatrix} L_{1} \\ Y_{1} \\ \vdots \\ L_{2} \\ P \end{bmatrix}_{p} \begin{bmatrix} L_{3} \\ Y_{2} \\ \vdots \\ R_{2} \end{bmatrix}_{q} \begin{bmatrix} L_{3} \\ Y_{2} \\ \vdots \\ R_{3} \end{bmatrix}$$

where R_2 , R_3 , L_1L_2 , L_3 , L_4 , Y_1 , Y_2 , Y_3 , o, p, q, and n each have the same meanings as R_2 , R_3 , L_1L_2 , L_{3a} , L_4 , Y_1 , Y_2 , Y_3 , o, p, q, and n in the formula (2).]

The polycyclic compound of the present invention represented by the general formula (1) or (2) has as a substituent a fused ring such as carbazole so that the polycyclic compound can increase Tg and improve thin film stability in the case of being formed into a device compared to the case of a compound having a substituent formed of a single ring. In addition, because the binding positions of the fused rings such as carbazole represented by $\rm L_1$ and $\rm L_2$ are the meta position, expansion of the conjugate system can be prevented and the triplet energy gap can be enlarged. On the contrary, when the binding positions of the fused rings such as carbazole are the para position, the conjugate system is expanded and the triplet energy gap may be reduced.

The case where the polycyclic compound of the present invention has the structure B represented by the following general formula (3c) or the general formulae (7-1) to (18-1) below is preferred, because the triplet energy gap can be enlarged as described above so that the binding positions of the fused rings such as carbazole represented by L_3 , L_{3a} , and L_{3b} are the meta position.

$$C_1 \underbrace{\begin{array}{c} Y_2 \\ C_2 \\ X_2 \end{array}}_{[L_{3b}]_r} [L_{3a}]_q$$

The polycyclic compound of the present invention is preferably represented by any one of the following general formulae (7) to (18):

[Chem 8]

[In the general formulae (7) to (10), X_3 , X_4 , X_5 , and X_6 each independently represent oxygen (O), sulfur (S), N—R₁, or CR₂R₃, and R₁, R₂, and R₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 60 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted or unsubstituted or unsubstituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the 65 aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic

ring, provided that when both X_3 and X_4 or both X_5 and X_6 represent N— R_1 , at least one R_1 represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring.

In the general formulae (7) to (10), o, p, and q each independently represent 0 or 1, provided that o+p is 1 or more.

In the general formulae (9) and (10), n represents 2, 3, or 4. In the general formulae (7) to (10), L_1 , L_2 , and L_3 each independently represent a structure represented by the gen-10 eral formula (4), Ar₁ and Ar₂ each independently represent a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, E represents a single bond, oxygen (O), sulfur (S), N—R₄, or CR₅R₆, R₄, R₅, and R₆ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsub-20 stituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic het-25 erocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formulae (9) and (10), when n represents 2, L₄ represents a single bond, oxygen (C), sulfur (S), CO, SO, PO, SO₂, N-R₇, a substituted or unsubstituted alkylene 30 group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aro-35 matic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, R7 represents a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group 45 having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, when n represents 3, L4 represents N, a substituted or unsubstituted alkanetriyl group having 1 to 20 carbon atoms, a substituted or 50 unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, and when n represents 4, L₄ represents a substituted or unsubstituted alkane tetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formulae (7) to (10), Y_1 , Y_2 , and Y_3 each independently represent a substituted or unsubstituted alkyl

group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having a 1 to 20 carbon atoms, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubsti- $\,^{\,5}$ tuted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, which is bonded with a carbon atom, the number of Y_1 's is 0, 1, 2, or 3, the number of Y_2 's is 0, 1, 2, 3, or 4, and the number of Y_3 's is 0, 1, or 2.]

As the polycyclic compounds represented by the above

general formulae (7) to (10), the compound represented by 15 any one of the following formulae (7-1), (7-2), (8-1), (8-2), (9-1), (9-2), (10-1), and (10-2) is preferred.

[Chem 9] 20 (7-1)

$$Y_1$$
 X_3
 Y_2
 X_4
 Y_2
 X_4

$$\begin{array}{c} \text{[L_1]}_o \\ \text{Y}_1 \\ \\ \text{[L_2]}_p \end{array} \\ \begin{array}{c} \text{X}_6 \\ \\ \text{Y}_3 \end{array} \\ \begin{array}{c} \text{Y}_2 \\ \\ \text{L}_3 \end{array} \end{array}$$

$$\begin{array}{c} \text{[L_1]}_o \\ \text{Y}_1 \\ \end{array} \begin{array}{c} \text{X}_6 \\ \end{array} \begin{array}{c} \text{L}_3 \\ \end{array} \begin{array}{c} \text{(8-2)} \\ \text{45} \\ \end{array}$$

$$\begin{bmatrix} \begin{bmatrix} L_1 \end{bmatrix}_o & Y_3 & Y_2 \\ Y_1 & & & \\ & & &$$

$$\begin{bmatrix} \begin{bmatrix} L_1 \end{bmatrix}_o & X_6 & L_3 \\ Y_1 & X_5 & Y_3 & Y_2 \end{bmatrix}_n L_4$$

[Chem 10]

25

30

35

40

$$Y_{2}$$

$$X_{3}$$

$$Y_{1}$$

$$X_{3}$$

$$Y_{3}$$

$$X_{4}$$

$$X_{5}$$

$$X_{8}$$

$$X_{8}$$

$$X_{1}$$

$$X_{2}$$

$$X_{3}$$

$$X_{4}$$

$$X_{5}$$

$$X_{6}$$

$$\begin{array}{c} Y_2 \\ X_{10} \\ Y_1 \\ X_9 \\ Y_3 \end{array}$$

$$\begin{array}{c} Y_2 \\ X_{12} \\ Y_1 \\ X_{12} \\ X_{12} \\ Y_3 \end{array}$$

$$\begin{bmatrix} X_1 & X_2 & X_3 \\ Y_1 & X_3 & X_4 \end{bmatrix}_{q} L_4$$

(15)

13

-continued

$$\begin{bmatrix} Y_2 & & & & \\ & & & & \\ & & & & \\ Y_1 & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

$$\begin{bmatrix} I_{L_1]_o} & & & & & & & \\ Y_1 & & & & & & & \\ Y_1 & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & \\ & & \\ & \\ & & \\$$

$$--$$
N $\stackrel{Ar_1}{\underset{Ar_2}{\bigvee}}$ E

[In the general formulae (11) to (16), X_7 , X_8 , X_9 , X_{10} , X_{11} , and X_{12} each independently represent oxygen (O), sulfur (S), $_{35}$ N—R₁, or CR₂R₃, R₁, R₂, and R₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a 40 substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, 45 provided that when both X_7 and X_8 , both X_9 and X_{10} , or both X_{11} and X_{12} represent N— R_1 , at least one R_1 represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring.

In the general formulae (11) to (16), o, p, and q each independently represent 0 or 1, provided that o+p is 1 or more. In the general formulae (14) to (16), n represents 2, 3, or 4.

In the general formulae (11) to (16), L_1 , L_2 , and L_3 each independently represent a structure represented by the general formula (7), Ar_1 and Ar_2 each independently represent a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, E_1 corpresents a single bond, oxygen (O), sulfur (S), E_2 0 represents a single bond, oxygen (O), sulfur (S), E_3 1 nor E_4 2, or E_4 3, and E_5 4, and E_6 4 each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted or unsubstitute

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bon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring

In the general formulae (14) to (16), when n represents 2, L₄ represents a single bond, oxygen (O), sulfur (S), CO, SO, PO, SO₂, N—R₇, a substituted or unsubstituted alkylene $_{10}$ group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aro-(16) 15 matic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, R7 represents a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, when n represents 3, L₄ represents N, a substituted or unsubstituted alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, and when n represents 4, L₄ represents a substituted or unsubstituted alkane tetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formulae (11) to (16), Y_1 , Y_2 , and Y_3 each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted or unsubstituted or unsubstituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, which is bonded with a carbon atom, the number of Y_1 's is 0, 1, 2, or 3, the number of Y_2 's is 0, 1, 2, 3, or 4, and the number of Y_3 's is 0, 1, or 2.]

As the polycyclic compounds represented by the above general formulae (11) to (16), the compound represented by any one of the following general formulae (11-1), (11-2), (12-1), (12-2), (13-1), (13-2), (14-1), (14-2), (15-1), (15-2), (16-1), and (16-2) is preferred.

[Chem 11]

$$\begin{array}{c} L_3 \\ Y_2 \\ X_7 \\ Y_1 \\ X_8 \end{array}$$

$$Y_2$$
 X_3
 X_1
 X_2
 X_3
 X_4
 X_8
 X_8
 X_8
 X_8
 X_8
 X_8
 X_8

$$\begin{array}{c} Y_2 \\ X_{10} \\ Y_1 \\ X_2 \\ Y_3 \end{array}$$

(12-2)

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$$Y_2$$
 X_{10}
 Y_1
 X_{10}
 X_{10}
 X_{10}
 X_{10}

$$\begin{array}{c} L_3 \\ Y_2 \\ X_{12} \\ X_{12} \\ X_{12} \\ X_{23} \\ X_{12} \\ X_{23} \\ X_{24} \\ X_{25} \\ X_$$

$$\begin{array}{c} Y_2 \\ X_{12} \\ X_{12} \\ X_{12} \\ X_{12} \\ X_{13} \\ X_{14} \\ X_{15} \\ X_{15} \\ X_{16} \\ X_{17} \\ X_{18} \\ X_{19} \\$$

$$\begin{bmatrix} L_3 \\ Y_2 \\ \vdots \\ Y_1 \\ \vdots \\ X_N \end{bmatrix}_n$$
 (14-1)

$$\begin{bmatrix} I_{-1} \\ Y_1 \\ \vdots \\ I_{-2} \\ P_3 \end{bmatrix} X_8$$

$$\begin{bmatrix} I_{-1} \\ X_8 \\ \vdots \\ X_8 \end{bmatrix}_n$$

$$(14-2)$$

$$\begin{bmatrix} X_1 & X_{10} & X_$$

(13-1) 55
$$L_3$$
 Y_2 L_4 Y_1 Y_2 X_{10} X_{10}

$$[L_1]_o \qquad \qquad Y_2 \\ [L_2]_p \qquad \qquad X_{13} \qquad \qquad X_{14}$$

$$\begin{bmatrix} L_1 \\ 0 \end{bmatrix}_p \\ X_{13} \\ X_{14} \\ X_{14} \\ X_{14} \\ X_{15} \\ X_{16} \\ X_{16} \\ X_{17} \\ X_{18} \\ X_{19} \\ X_{$$

$$--N \underbrace{\stackrel{Ar_1}{\bigwedge}}_{Ar_2} E$$
(4)

[In the general formulae (17) and (18), X_{13} and X_{14} each independently represent oxygen (O), sulfur (S), N-R₁, or CR₂R₃, R₁, R₂, and R₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon 55 atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic 60 hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, provided that when both X_{13} and X_{14} represent N— R_1 , at least one R_1 represents a substituted or unsubstituted 65monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring.

In the general formulae (17) and (18), o, p, and q each independently represent 0 or 1, provided that 0+p is 1 or more. In the general formula (18), n represents 2, 3, or 4.

In the general formulae (17) and (18), L_1 , L_2 , and L_3 each independently represent a structure represented by the general formula (3), Ar₁ and Ar₂ each independently represent a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring or a substituted or unsubstituted divalent aromatic heterocy-10 clic group having 3 to 24 atoms forming the aromatic ring, E represents a single bond, oxygen (O), sulfur (S), N-R₄, or CR₅R₆, R₄, R₅, and R₆ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 15 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the 20 aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic

In the general formula (18), when n represents 2, L₄ represents a single bond, oxygen (C), sulfur (S), CO, SO, PO, 25 SO₂, N—R₇, a substituted or unsubstituted alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon 30 atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, R7 represents a substituted or unsubstituted alkyl group (18) 35 having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubsti-40 tuted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, when n represents 3, L4 represents N, a substituted or unsubstituted alkanetriyl group having 1 to 45 20 carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, a substituted or unsubstituted trivalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, and when n represents 4, L₄ represents a substituted or unsubstituted alkane tetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formulae (17) and (18), Y_1, Y_2 , and Y_3 each independently represent an alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted or unsu

(18-1)

ing 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms which is bonded with a carbon atom forming the aromatic ring, the 5 number of Y_{1} 's is 0, 1, 2, or 3, the number of Y_{2} 's is 0, 1, 2, 3, or 4, and the number of Y_{3} 's is 0, 1, or 2.]

As the polycyclic compounds represented by the above general formulae (17) and (18), the compound represented by any one of the following formulae (17-1), (17-2), (18-1), and (18-2) is preferred.

$$\begin{bmatrix} L_1 \end{bmatrix}_{p}$$

$$\begin{bmatrix} L_2 \end{bmatrix}_{p}$$

$$X_{13}$$

$$X_{14}$$

$$\begin{array}{c} X_{1} \\ Y_{1} \\ X_{13} \end{array}$$

$$\begin{bmatrix} L_1 \\ p \end{bmatrix}_p$$

$$\begin{bmatrix} L_1 \\ Y_1 \end{bmatrix}$$

$$X_{13}$$

$$X_{14}$$

$$X_{14}$$

$$\begin{bmatrix} L_1 \\ V_1 \\ L_2 \end{bmatrix}_p$$

$$X_{13}$$

$$X_{14}$$

$$Y_2$$

$$X_{14}$$

$$X_{14}$$

$$Y_3$$

$$X_{14}$$

In addition, the polycyclic compound represented by the above general formula (8) is preferably the polycyclic compound represented by the following general formula (19). The polycyclic compound represented by the above general formula (10) is preferably the compound represented by the following general formula (20).

$$\begin{bmatrix} L_1 \\ V_1 \\ \vdots \\ L_2 \\ D \end{bmatrix} = \begin{bmatrix} L_3 \\ V_2 \end{bmatrix}$$

In the general formulae (1), (2), (3b), and (7) to (18) X_1 to X_{14} each independently represent oxygen (O), sulfur (S), N—R₁, or CR₂R₃ (N—R₁ or CR₂R₃ bonds to the benzene ring to which the N atom or the C atom is adjacent).

In the general formulae (1), (2), and (7) to (18), R_1 , R_2 , and R₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 35 atoms forming the aromatic ring, provided that when both X_1 and X_2 represent N— R_1 , when both X_3 and X_4 represent $N-R_1$, when both X_5 and X_6 represent $N-R_1$, when both X_7 and X_8 represent N— R_1 , when both X_9 and X_{10} represent N— R_1 , when both X_{11} and X_{12} represent N— R_1 , and when both X_{13} and X_{14} represent N— R_1 , at least one R_1 represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring

In the general formulae (1), (2), and (7) to (18), Y_1 , Y_2 , and Y_3 each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted or unsubstituted or unsubstituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 carbon atoms forming the aromatic ring, the number of Y_1 's is 0, 1, 2, or 3, the number of Y_2 's is 0, 1, 2, or 3, or 4, and the number of Y_3 's is 0, 1, or 2.

In the general formulae (1), (2), and (7) to (18), L₁, L₂, L₃, 60 L_{3a}, and L_{3b} each independently represent a structure represented by the general formula (4).

In the general formula (4), Ar_1 and Ar_2 each independently represent a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring or a substituted or unsubstituted divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

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In the general formula (4), E represents a single bond, oxygen (O), sulfur (S), N—R₄, or CR_5R_6 , and R_4 , R_5 , and R_6 each independently a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the 5 ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted or group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring (N—R₄ or CR_5R_6 bonds to the benzene ring to which the N atom or the C atom is adjacent).

In the general formulae (2), (9), (10), (14) to (16), (18), and (20), n represents 2, 3, or 4.

In the general formulae (2), (9), (10), (14) to (16), (18), and (20), when n represents 2, L₄ represents a single bond, oxygen (O), sulfur (S), CO, SO, PO, SO₂, N—R₇, a substituted or unsubstituted alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 20 carbon atoms forming the ring, a substituted or unsubstituted divalent organosilyl group having 2 to 20 carbon atoms, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocy- 25 clic group having 3 to 24 atoms forming the aromatic ring, R₇ represents a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted aralkyl group having 7 to 24 carbon 30 atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, when n repre- 35 sents 3, L₄ represents N, a substituted or unsubstituted trivalent alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted trivalent cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted trivalent organosilyl group having 1 to 20 car- 40 bon atoms, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, and when n represents 4, L₄ represents a sub- 45 stituted or unsubstituted tetravalent alkane tetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted tetravalent cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 50 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring.

In the general formulae (1), (2), and (7) to (18), 0, p, and q each represent 0 or 1, provided that 0+p is 1 or more.

Examples of the alkyl group having 1 to 20 carbon atoms and represented by Y_1 to Y_3 and R_1 to R_7 include a methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl group, an s-butyl group, a t-butyl group, an isobutyl group, an n-pentyl group, an n-hexyl group, an n-heptyl 60 group, an n-octyl group, an n-nonyl group, an n-tridecyl group, an n-tetradecyl group, an n-pentadecyl group, an n-hexadecyl group, an n-heptadecyl group, an n-octadecyl group, an neopentyl group, a 1-methylpentyl group, a 2-methylpentyl group, a 1-heptyloctyl group, and a 3-methylpentyl group. Preferred are a

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methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl group, an s-butyl group, an isobutyl group, a t-butyl group, n-pentyl group, an n-hexyl group, an n-heptyl group, an n-octyl group, an n-nonyl group, an n-decyl group, an n-undecyl group, an n-dodecyl group, an n-tridecyl group, an n-tetradecyl group, an n-pentadecyl group, an n-hexadecyl group, an n-heptadecyl group, an n-octadecyl group, an neopentyl group, a 1-methylpentyl group, a 1-pentylhexyl group, a 1-butylpentyl group, and a 1-heptyloctyl group.

Examples of the cycloalkyl group having 3 to 20 carbon atoms forming the ring and represented by Y_1 to Y_3 and R_1 to R_7 include a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group. Preferred are a cyclobutyl group, a cyclopentyl group, and a cyclohexyl group.

Examples of the alkoxy group having 1 to 20 carbon atoms and represented by Y_1 to Y_3 include a methoxy group, an ethoxy group, a methoxy group, an i-propoxy group, an n-propoxy group, an n-butoxy group, an s-butoxy group, and a t-butoxy group. Preferred are a methoxy group, an ethoxy group, a methoxy group, an i-propoxy group, and an n-propoxy group.

Examples of the aralkyl group having 7 to 24 carbon atoms and represented by Y_1 to Y_3 and R_1 to R_7 include a benzyl group, a phenethyl group, and a phenylpropyl group.

Examples of the organosilyl group having 1 to 20 carbon atoms and represented by Y_1 to Y_3 and R_1 to R_7 include a trimethyl silyl group, a triethyl silyl group, a tributyl silyl group, a tributyl silyl group, a dimethylethyl silyl group, a dimethylisopropyl silyl group, a dimethylpropyl silyl group, a dimethylbutyl silyl group, a dimethyltertiary butyl silyl group, a diethylisopropyl silyl group, a phenyldimethyl silyl group, a diphenyl tertiary butyl group, and a triphenyl silyl group. Preferred are a trimethyl silyl group, a triethyl silyl group, and a tributyl silyl group.

Examples of the aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring and represented by Y_1 to Y_3 and R_1 to R_7 include monovalent residues such as benzene, naphthalene, biphenyl, terphenyl, fluorene, phenanthrene, triphenylene, perylene, chrysene, fluoranthene, benzofluorene, benzotriphenylene, and benzochrysene. Preferred are monovalent residues such as benzene, naphthalene, biphenyl, terphenyl, fluorene, and phenanthrene. Examples of the divalent aromatic hydrocarbon group having 6 to 24 carbon atoms and represented by Ar_1 and Ar_2 include divalent residues such as benzene, naphthalene, biphenyl, terphenyl, fluorene, phenanthrene, triphenylene, perylene, chrysene, fluoranthene, benzofluorene, bnezotriphenylene, and benzochrysene. Preferred are divalent residues such as benzene, biphenyl, terphenyl, fluorene, and phenanthrene.

Examples of the aromatic heterocyclic group having 3 to 24 carbon atoms forming the aromatic ring and represented by Y_1 to Y_3 and R_1 to R_7 include monovalent residues such as pyridine, pyridazine, pyrimidine, pyrazine, 1,3,5-triazine, carbazole, dibenzofuran, dibenzothiophene, phenoxazine, phenothiazine, and dihydroacridine. Preferred are monovalent residues such as carbazole, dibenzofuran, dibenzothiophene, phenoxazine, and dihydroacridine. Further, examples of the monovalent fused aromatic heterocyclic group having 8 to 24 carbon atoms forming the aromatic ring and represented by at least one R₁ include compounds having fused structures of those examples. Examples of the aromatic heterocyclic group having 3 to 24 carbon atoms forming the aromatic ring and represented by Ar₁ and Ar₂ include divalent residues such as pyridine, pyridazine, pyrimidine, pyrazine, 1,3,5-triazine, carbazole, dibenzofuran, dibenzothiophene, 23

phenoxazine, and phenothiazine. Preferred are divalent residues such as pyridine, pyridazine, pyrimidine, and pyrazine.

Examples of: when n indicated by L₄ represents 2, the alkylene group having 1 to 20 carbon atoms, the cycloalkylene group having 3 to 20 carbon atoms forming the ring, the divalent organosilyl group having 2 to 20 carbon atoms, the divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or the divalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring; when n represents 3, the alkanetrivl group having 1 to 20 10 carbon atoms, the cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, the trivalent organosilyl group having 1 to 20 carbon atoms, the trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or the trivalent aromatic heterocyclic group having 3 to 15 24 atoms forming the aromatic ring; and when n represents 4, the alkane tetrayl group having 1 to 20 carbon atoms, the cycloalkane tetrayl group having 3 to 20 carbon atoms forming the ring, the tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or the 20 tetravalent aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring include divalent to tetravalent groups of the corresponding groups described in Y₁ to Y₃ and

Examples of the substituent that can be substituted for the 25 each group in the general formulae (1), (2), and (7) to (18) include alkyl groups each having 1 to 10 carbon atoms (such as a methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl group, an s-butyl group, an isobutyl group, a t-butyl group, an n-pentyl group, an n-hexyl group, 30 an n-heptyl group, an n-octyl group, a hydroxymethyl group, a 1-hydroxyethyl group, a 2-hydroxyethyl group, a 2-hydroxyisobutyl group, a 1,2-dihydroxyethyl group, a 1,3-dihydroxyisopropyl group, a 2,3-dihydroxy-t-butyl group, a 1,2, 3-trihydroxypropyl group, a chloromethyl group, a 35 1-chloroethyl group, a 2-chloroethyl group, a 2-chloroisobutyl group, a 1,2-dichloroethyl group, a 1,3-dichloroisopropyl group, a 2,3-dichloro-t-butyl group, a 1,2,3-trichloropropyl group, a bromomethyl group, a 1-bromoethyl group, a 2-bromoethyl group, a 2-bromoisobutyl group, a 1,2-dibromoethyl 40 group, a 1,3-dibromoisopropyl group, a 2,3-dibromo-t-butyl group, a 1,2,3-tribromopropyl group, a iodomethyl group, a 1-iodoethyl group, a 2-iodoethyl group, a 2-iodoisobutyl group, a 1,2-diiodoethyl group, a 1,3-diiodoisopropyl group, a 2,3-diiodo-t-butyl group, a 1,2,3-triiodopropyl group, an 45 aminomethyl group, a 1-aminoethyl group, a 2-aminoethyl group, a 2-aminoisobutyl group, a 1,2-diaminoethyl group, a 1,3-diaminoisopropyl group, a 2,3-diamino-t-butyl group, a 1,2,3-triaminopropyl group, a cyanomethyl group, a 1-cyanoethyl group, a 2-cyanoethyl group, a 2-cyanoisobutyl 50 group, a 1,2-dicyanoethyl group, 1,3-dicyanoisopropyl group, a 2,3-dicyano-t-butyl group, a 1,2,3-tricyanopropyl group, a nitromethyl group, a 1-nitroethyl group, a 2-nitroethyl group, a 2-nitroisobutyl group, a 1,2-dinitroethyl group, a 1,3-dinitroisopropyl group, a 2,3-dinitro-t-butyl group, and a 55 1,2,3-trinitropropyl group), cycloalkyl groups each having 3 to 40 carbon atoms forming the ring (such as a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, a 4-methylcyclohexyl group, a 1-adamantyl group, a 2-adamantyl group, a 1-norbornyl group, and a 2-norbornyl 60 group), alkoxy groups each having 1 to 6 carbon atoms (such as an ethoxy group, a methoxy group, an i-propoxy group, an n-propoxy group, an s-butoxy group, a t-butoxy group, a pentoxy group, and a hexyloxy group), cycloalkoxy groups each having 3 to 10 carbon atoms forming the ring (such as a 65 cyclopentoxy group and a cyclohexyloxy group), aromatic hydrocarbon groups each having 6 to 40 carbon atoms form24

ing the aromatic ring, aromatic heterocyclic groups having 3 to 40 atoms forming the aromatic ring, amino groups substituted with aromatic hydrocarbon groups having 6 to 40 carbon atoms forming the aromatic ring, ester groups having aromatic hydrocarbon groups having 6 to 40 carbon atoms forming the aromatic ring, an ester group, cyano group, nitro group, and halogen atom, each of which has an alkyl group having 1 to 6 carbon atoms.

Of those, alkyl groups each having 1 to 6 carbon atoms, a phenyl group, a pyridyl group, a carbazolyl group, and a dibenzofuranyl group are preferred and the number of substituents is preferably 1 or 2.

The total number of the substituents represented by Y_1, Y_2 , and Y_3 in the general formulae (1), (7), (8), (11), (12), (13), (17), and (19) is preferably 2 or less, or the total number of the substituents represented by Y_1, Y_2 , and Y_3 with respect to one structure inside []_n in the general formulae (2), (9), (10), (14), (15), (16), (18), and (20) is preferably 2 or less, the number of the substituents represented by Y_1 and Y_2 is more preferably 0, or the number of the substituents represented by Y_3 is more preferably 0.

In the general formulae (1), (2), and (7) to (18), o+p+q is preferably 2 or less and o+p is more preferably 1.

In the polycyclic compound of the present invention, both X_1 and X_2 , both X_3 and X_4 , both X_5 and X_6 , both X_7 and X_8 , both X_9 and X_{10} , both X_{11} and X_{12} , and both X_{13} and X_{14} in the general formulae (1), (2), (7) to (18) are preferably compounds represented by N—R₁. A polycyclic compound in which X_1 to X_{14} represent N—R₁ has excellent hole transportability, and therefore, can prompt driving of an organic EL device at a low voltage, and in particular, can be used suitably as a host material or a hole transporting material.

At least one R₁ preferably represents a substituted or unsubstituted fused aromatic heterocycle having 8 to 24 atoms forming the aromatic ring and all of R₁'s more preferably represent fused aromatic heterocycles each having 8 to 24 atoms forming the aromatic ring. By bonding the fused aromatic heterocycle having electron transportability such as dibenzofuran and carbazole, the stability with respect to the hole (oxidation resistance) is enhanced compared that of a nitrogen-containing heterocycle which is not fused ring such as pyrimidine, resulting in long lifetime of the organic EL device. In addition, by bonding a fused aromatic heterocycle having large energy gap and the electron transportability such as dibenzofuran and carbazole to N, the degradation of the efficiency is prevented and the stability with respect to the hole (oxidation resistance) is enhanced in the case of using the organic EL device as a phosphorescence device.

Further, it is preferred that X_1 and X_2 in the general formulae (1) and (2) be each represented by N—R₁, and N—R₁ of X_1 and N—R₁ of X_2 be different from each other.

It is preferred that X_3 and X_4 , X_5 and X_6 in the general formulae (7) to (10) be each represented by N—R₁, and N—R₁ of X_3 and N—R₁ of X_4 or N—R₁ of X_5 and N—R₁ of X_6 be different from each other.

It is preferred that X_7 and X_8 , X_9 and X_{10} , X_{11} and X_{12} in the general formulae (11) to (16) be each represented by N—R $_1$, and N—R $_1$ of X_7 and N—R $_1$ of X_8 , N—R $_1$ of X_9 and N—R $_1$ of X_{10} , or N—R $_1$ of X_{11} and N—R $_1$ of X_{12} be different from each other.

It is preferred that X_{13} and X_{14} in the general formulae (17) and (18) be each represented by $N-\!\!\!-\!\!R_1$, and $N-\!\!\!-\!\!R_1$ of X_{13} and $N-\!\!\!-\!\!R_1$ of X_{14} be different from each other.

Thus, in the case where the structures in the formulae (1), (2), and (7) to (18) are asymmetric, crystallization thereof is suppressed and the stability of the thin film is enhanced,

whereby the lifetime of the device is improved compared to the case of symmetric structure.

In the polycyclic compound of the present invention, it is preferred that at least one of X_1 and X_2 in the general formulae (1) and (2) represent an oxygen atom, and it is more preferred that both X1 and X2 represent oxygen atoms. It is preferred that at least one of X₃ and X₄ in the general formulae (7) and (9) represent an oxygen atom, and it is more preferred that both X_3 and X_4 represent oxygen atoms. It is preferred that at 10 least one of X_5 and X_6 in the general formulae (8) and (10) represent an oxygen atom, and it is more preferred that both X₅ and X₆ represent oxygen atoms. It is preferred that at least one of X_7 and X_8 in the general formulae (11) and (14) represent an oxygen atom, and it is more preferred that both X₇ and X₈ represent oxygen atoms. It is preferred that at least one of X_9 and X_{10} in the general formulae (12) and (15) represent an oxygen atom, and it is more preferred that both $\rm X_9$ and $\rm X_{10}$ represent oxygen atoms. It is preferred that at least $\rm ^{20}$ one of X_{11} and X_{12} in the general formulae (13) and (16) represent an oxygen atom, and it is more preferred that both X_{11} and X_{12} represent oxygen atoms. It is preferred that at least one of X_{13} and X_{14} in the general formulae (17) and (18) 25 represent an oxygen atom, and it is more preferred that both X_{13} and X_{14} represent oxygen atoms. Because the oxygen atom has high electronegativity and can improve the electron transportability, the polycyclic compound of the present 30 invention in which X₁ to X₁₄ represent oxygen atoms can prompt the driving of the organic EL device at a low voltage and can be suitably used as a host material or an electron transporting material. When both X_1 and X_2 , both X_3 and X_4 , both X_5 and X_6 , both X_7 and X_8 , both X_9 and X_{10} , both X_{11} and X_{12} , and both X_{13} and X_{14} represent oxygen atoms, the triplet energy gap can be enlarged, and hence, the luminous efficiency can be improved compared to the case where both of them represent $N-R_1$ or both of them represent CR_2R_3 .

In addition, as the polycyclic compound of the present invention, a polycyclic compound represented by the general formula (7) or (9) in which both X₃ and X₄ represent CR₂R₃, a polycyclic compound represented by the general formula (13) or (16) in which both X₁₁ and X₁₂ represent CR₂R₃, and 45 a polycyclic compound represented by the general formula (17) and (18) in which both X₁₃ and X₁₄ represent CR₂R₃ are preferred. In those polycyclic compounds, the directions of two C (carbon atoms) are the same with respect to the ring A in the center of the molecule, the triplet energy gap can be enlarged slightly compared to the case where the directions of C (carbon atoms) are inverse, whereby the luminous efficiency can be improved.

Of those polycyclic compounds of the present invention, in the case of a compound represented by the general formula 55 (7), (9), (13), or (16) in which X_3 and X_4 or X_{11} and X_{12} are positioned at the same side with respect to the central benzene ring (ring A in the general formula (1)), the triplet energy gap can be enlarged slightly compared to the case where those are positioned at the inverse side, whereby the luminous efficiency can be improved. The same holds true in the case where X_3 and X_4 or X_{11} and X_{12} represent CR_2R_3 .

Of the polycyclic compounds of the present invention, the compounds represented by the general formulae (11) to (16) have both terminal benzene rings linked at the meta position 65 with respect to the central ring A, and therefore, can enlarge the triplet energy gap and have excellent luminous efficiency.

Of the polycyclic compounds of the present invention, the compounds represented by the general formulae (7) to (10) have both terminal benzene rings linked at the para position with respect to the central ring A, and therefore, have excellent electron transportability and can prompt driving of the organic EL device at a low voltage. Further, because the directions of X_3 and X_4 are the same with respect to the central ring A, the triplet energy gap can be enlarged, whereby the polycyclic compounds are excellent in the luminous efficiency.

The structure represented by the general formula (4) preferably has a structure selected from the structures represented by the following general formulae (21) to (39). The following structures may have substituents. Me represents a methyl group.

[Chem 16]

$$-N$$

$$-N$$

Specific examples of polycyclic compound represented by any one of the general formulae (1), (2), (7) to (20) of the

present invention are shown below. However, the present invention is not limited to these exemplified compounds.

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[Chem 19]

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[Chem 22]

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[Chem 23]

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[Chem 24]

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N & & & \\
N & \\
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[Chem 25]

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(1-146) \\
N \\
O \\
S
\end{array}$$

[Chem 26]

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(1-151) N N N

[Chem 27]

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[Chem 28]

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[Chem 30]

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[Chem 32]

[Chem 33]

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$$(1-252) \qquad (1-253)$$

[Chem 34]

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-continued (2-13)

$$(2-13) \qquad (2-14)$$

$$N \qquad (2-15) \qquad (2-16)$$

$$(2-19)$$

[Chem 35]

$$(2.20)$$

$$(2.22)$$

$$(2.22)$$

$$(2.23)$$

$$(2.24)$$

$$(2.24)$$

$$(2.24)$$

[Chem 36]

$$(2-39) \qquad (2-40)$$

$$(2-41)$$

$$(2-42)$$

$$(2-43)$$

$$\begin{array}{c} (2.43) \\ \\ \\ \\ \\ \\ \end{array}$$

$$(2-44)$$

$$(2-45)$$

$$(2-45)$$

[Chem 37]

(2-61)

(2-68)

[Chem 39]

-continued (2-86)

$$(2-90) \qquad (2-91)$$

-continued (2-92)

[Chem 40]

-continued (2-103)

-continued (2-111)

$$(2-117) \qquad (2-118)$$

$$(2-119) \qquad (2-120)$$

[Chem 42]

[Chem 43]

-continued (2-153)

[Chem 44]

$$(2-165)$$

$$(2-166)$$

[Chem 45]

$$(2-169) \qquad (2-170)$$

-continued (2-177)

[Chem 46]

$$(2-181)$$

$$(2-182)$$

$$(2-182)$$

$$(3-182)$$

$$(2-182)$$

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$$(3-182)$$

$$(3-182)$$

$$(3-182)$$

$$(3-1$$

[Chem 47]

$$(2-189) \qquad (2-190)$$

[Chem 48]

-continued (3-11)

[Chem 49]

(3-34)

[Chem 51]

(3-49)

-continued

(3-48)

[Chem 51]

[Chem 52]

(3-74)

[Chem 53]

-continued (3-81)

[Chem 54]

$$\begin{array}{c} (3\text{-}101) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}$$

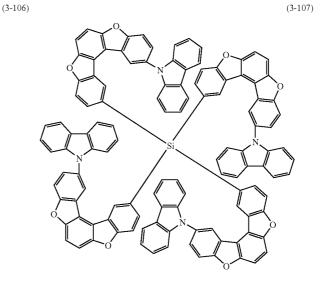
[Chem 55]

(3-104)

(3-105)

199 200

-continued



(3-108)

Indenofluorene (crosslinked with a carbon atom)

Next, an organic EL device of the present invention is described.

The organic EL device of the present invention has one or more organic thin film layers including a light emitting layer between a cathode and an anode, and at least one layer of the 50 organic thin film layers contains the polycyclic compound.

The polycyclic compound is contained in at least one layer of the organic thin film layers of the organic EL device of the present invention. In particular, in the case where the polycyclic compound is used as a material involved in the host 55 material or the electron transporting layer in the light emitting layer, higher luminous efficiency and longer lifetime of the device can be expected. In addition, in the case where the polycyclic compound is used as a material involved in the electron transport, the organic thin film layer preferably further includes, as a host material, a polycyclic compound having a π -conjugated heteroacene skeleton crosslinked with a carbon atom, a nitrogen atom, an oxygen atom, or a sulfur atom (hereinafter, may be abbreviated as π -conjugated heteroacene compound).

Specific examples of the π -conjugated heteroacene skeleton are described below, but are not limited thereto.

[Chem 57]

-continued

Indolocarbazole (crosslinked with a nitrogen atom)

Benzofuranodibenzofuran (crosslinked with an oxygen atom)

Benzothiophenodibenzothiophene (crosslinked with a sulfur atom)

45

50

55

60

In addition to the foregoing, a π -conjugated heteroacene skeleton crosslinked with a combination of a carbon atom, a 20 nitrogen atom, an oxygen atom, and a sulfur atom is also permitted. Specific examples of the π -conjugated heteroacene skeleton are shown below.

[Chem 60]

The polycyclic compound of the present invention may have an electron transporting layer between the light emitting layer and the cathode, and the electron transporting layer may contain the polycyclic compound of the present invention. 65 Further, the light emitting layer preferably contains the π -conjugated heteroacene compound.

Alternatively, the polycyclic compound may have a hole transporting layer between the light emitting layer and the anode, and the hole transporting layer may contain the polycyclic compound of the present invention.

Further, in the case where the polycyclic compound of the present invention is used in the electron transporting layer or an electron injecting layer, the organic light emitting device can be driven under a low voltage. In addition, the π-conjugated heteroacene compound is preferably included in the light emitting layer and in the case where the π-conjugated heteroacene compound is used as a light emitting layer, the long lifetime of the organic EL device can be obtained. The case where the polycyclic compound is included in the electron transporting layer or the electron injecting layer and the mitting layer simultaneously is preferred because the organic EL device can be driven at a low voltage and the long lifetime thereof can be obtained.

In particular, the light emitting layer preferably includes a π -conjugated heteroacene compound as a host material, more preferably a π-conjugated heteroacene compound represented by any one of the following general formulae (40) to (43), still more preferably a π -conjugated heteroacene compound represented by any one of the following general formulae (44) to (47), and particularly preferably a π -conjugated heteroacene compound represented by the following general formula (44) or (45). The case where the π -conjugated heteroacene compound represented by any one of the general formulae (40) to (47) is included as a host material is pre-30 ferred, because the crosslinking part of the heteroacene skeleton is directed in the same direction with respect to the central benzene ring, and hence the triplet energy gap can be enlarged and the luminous efficiency can be improved compared to the case where the direction is inverse. In particular, in the general formulae (40) to (43), it is preferred that at least one of X_{15} and X_{16} represent an oxygen atom and it is more preferred that both of them represent oxygen atoms. This is because the oxygen atom has high electronegativity, and hence can improve electron transportability and prompt the 40 driving of the device at a low voltage, and can be suitably used as an electron transporting material.

[Chem 61]

$$\begin{array}{c}
Y_2 \\
X_{1} \\
Y_1
\end{array}$$

$$\begin{array}{c}
X_{2} \\
X_{16}
\end{array}$$

$$\begin{array}{c}
X_{2} \\
X_{3}
\end{array}$$

$$\begin{array}{c}
X_{2} \\
X_{3}
\end{array}$$

$$\begin{array}{c}
X_{16} \\
X_{18}
\end{array}$$

$$\begin{array}{c}
X_{18} \\
X_{18}
\end{array}$$

$$\begin{array}{c}
X_{18} \\
X_{18}
\end{array}$$
(41)

[In the formulae (40) to (43), X_{15} , X_{16} , X_{17} and X_{18} each independently represent oxygen (C), sulfur (S), N—R₁, or CR₂R₃. R₁, R₂, and R₃ each independently represent an alkyl group having 1 to 20 carbon atoms, a substituted or unsubsti-

tuted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an aralkyl group having 7 to 24 carbon atoms, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or sunsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, provided that when both X_{15} and X_{16} , or both X_{17} and X_{18} represent N—R₁, at least one R₁ represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring.

In the formulae (42) and (43), n represents 2, 3, or 4, and the material represented by the formulae (42) and (43) includes a dimer using L_3 as a linking group for n=2, a trimer using L_3 as a linking group for n=3, or a tetramer using L_3 as a linking 15 group for n=4.

In the formulae (40) to (43), L_1 represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 20 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring 25 and which is linked with a benzene ring a through a carbon-carbon bond.

In the formulae (40) and (41), L_2 represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon 30 atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carboncarbon bond, provided that when both X_{15} and X_{16} , or both X_{17} and X_{18} represent CR_2R_3 and both L_1 and L_2 represent substituted or unsubstituted divalent aromatic hydrocarbon 40 groups each having 6 to 24 carbon atoms forming the aromatic ring, a case where L_1 and L_2 are simultaneously linked at para position with respect to a benzene ring b is excluded.

In the formulae (42) and (43), when n represents 2, L_3 represents a single bond, an alkylene group having 1 to 20 45 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon 50 atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with a benzene ring c through a carbon-carbon bond, when n represents 3, L₃ represents an alkanetriyl group having 1 to 20 55 free of any carbonyl group.] carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the aromatic ring, a trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group which has 3 to 24 atoms and which is linked with a benzene ring c through a carbon-carbon bond, or when n represents 4, L₃ represents an alkanetetrayl having 1 to 20 carbon atoms, a 65 substituted or unsubstituted cycloalkanetetrayl having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or

unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carbon-carbon bond, provided that when both $\rm X_{15}$ and $\rm X_{16}$ or both $\rm X_{17}$ and $\rm X_{18}$ represent $\rm CR_2R_3$ and both $\rm L_1$ and $\rm L_3$ represent substituted or unsubstituted divalent, trivalent, or tetravalent aromatic hydrocarbon groups each having 6 to 24 carbon atoms forming the aromatic ring, a case where $\rm L_1$ and $\rm L_3$ are simultaneously linked at para position with respect to the benzene ring b is excluded.

In the formulae (40) to (43), A_1 represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with L_1 through a carbon-carbon bond, provided that when L_1 represents an alkyl or alkylene group having 1 to 20 carbon atoms, a case where A_1 represents a hydrogen atom is excluded.

In the formulae (40) and (41), A_2 represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with L_2 through a carbon-carbon bond, provided that when L_2 represents an alkyl or alkylene group having 1 to 20 carbon atoms, a case where A_2 represents a hydrogen atom is excluded.

In the formulae (40) to (43), Y_1 , Y_2 , and Y_3 each represent an alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an alkoxy group having 1 to 20 carbon atoms, an aralkyl group having 7 to 24 carbon atoms, a organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring a, b, or c through a carbon-carbon bond, the number of each of Y_1 and Y_3 is 0, 1, 2, or 3, and the number of Y_2 is 0, 1, or 2, provided that when both X_{15} and X_{16} or both X_{17} and X_{18} represent oxygen (C), sulfur (S), or CR_2R_3 , L_1 and L_2 represent single bonds, and both A_1 and A_2 represent hydrogen atoms, a case where a benzene ring b has one or two Y₂'s, which represent a methyl group or an unsubstituted phenyl group is excluded.

In the formulae (40) to (43), A_1 , A_2 , L_1 , L_2 , and L_3 are each free of any carbonyl group.

$$Y_1$$
 A_1
 A_1
 A_1
 A_1
 A_1
 A_1
 A_1
 A_1
 A_2
 A_2
 A_2
 A_2
 A_3
 A_4
 A_1
 A_2
 A_3
 A_4
 A_4
 A_4
 A_5
 A_5

$$\begin{bmatrix} A_1 & L_1 & & & \\$$

$$\begin{bmatrix} A_1 \\ Y_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_7 \\ A_8 \\ A_$$

[In the formulae (45) and (47), n represents 2, 3, or 4, and the material represented by any one of the formulae (45) to (47) includes a dimer using L_3 as a linking group for n=2, a trimer using L_3 as a linking group for n=3, or a tetramer using L_3 as a linking group for n=4.

In the formulae (44) to (47), L_1 represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with a benzene ring a through a carbon-carbon bond.

In the formulae (44) and (45), L_2 represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon 55 atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with a benzene ring c through a carbon-carbon bond.

In the formulae (46) and (47), when n represents 2, L_3 represents a single bond, an alkylene group having 1 to 20 $\,$ 65 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent

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organosilyl group having 2 to 20 carbon atoms, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carbon-carbon bond, when n represents 3, L₃ represents an alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group which has 3 to 24 atoms and which is linked with the benzene ring c through a carbon-carbon bond, or when n represents 4, L₃ represents an alkanetetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carbon-carbon bond.

In the formulae (44) to (47), A_1 represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with L_1 through a carbon-carbon bond, provided that when L_1 represents an alkyl or alkylene group having 1 to 20 carbon atoms, a case where A_1 represents a hydrogen atom is excluded.

In the formulae (44) and (45), A_2 represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with L_2 through a carbon-carbon bond, provided that when L_2 represents an alkyl or alkylene group having 1 to 20 carbon atoms, a case where A_2 represents a hydrogen atom is excluded.

In the formulae (44) to (47), Y_1 , Y_2 , and Y_3 each represent an alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an alkoxy group having 1 to 20 carbon atoms, an aralkyl group having 7 to 24 carbon atoms, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring a, b, or c through a carbon-carbon bond, the number of each of Y₁ and Y₃ is 0, 1, 2, or 3, and the number of Y_2 is 0, 1, or 2, provided that when both L_1 and L_2 represent single bonds, and both A_1 and A_2 represent hydrogen atoms, a benzene ring b has one or two Y2's, which represent a methyl group or an unsubstituted phenyl group is excluded.

In the formulae (44) to (47), A, A₂, L₁, L₂, and L₃ are each free of any carbonyl group.]

In the formulae (40) to (47), examples of each group represented by Y_1 to Y_3 , R_1 to R_3 , L_1 to L_3 , and A_1 to A_2 and the substituent thereof include the same examples exemplified for the formulae (1) to (20).

Specific examples of the π -conjugated heteroacene compound represented by the formulae (40) to (47) of the present invention are described below, but are not limited to those exemplified compounds.

[Chem 63]

$$(4.8)$$

[Chem 64]

[Chem 65]

$$(4-28)$$

(4-39)

[Chem 67]

$$(4.52)$$

$$N = N$$

$$N =$$

[Chem 68]

[Chem 69]

$$(4-78)$$

[Chem 70]

(4-102)

(4-107)

-continued (4-101)

[Chem 71]

[Chem 72]

$$\bigcap_{S} S = \bigcap_{S} S$$

[Chem 73]

[Chem 74]

[Chem 75]

[Chem 77]

$$(4.161)$$

[Chem 79]

(4-185)

-continued (4-186)

[Chem 80]

-continued (4-204)

[Chem 81]

$$(4-207) \qquad (4-208)$$

-continued (4-211)

-continued [Chem 82]

-continued (4-220)

[Chem 83]

[Chem 84]

[Chem 85]

$$(4-267)$$

[Chem 91]

$$(4-327)$$

$$N$$

$$N$$

$$(4-329)$$

$$N$$

$$N$$

$$(4-330)$$

$$(4-332)$$

$$(4-333)$$

$$(4-334)$$

[Chem 92]

$$(4.344) \qquad (4.345)$$

$$(4.350)$$

$$(4.351)$$

$$(4.352)$$

(4-359)

-continued

Examples of the structure of the multi-layered organic EL device include layered multi-layer constitutions such as anode/hole transporting layer (hole injecting layer)/light emitting layer/cathode, anode/light emitting layer/electron transporting layer (electron injecting layer)/cathode, anode/hole transporting layer (hole injecting layer)/light emitting layer/electron transporting layer (electron injecting layer)/cathode, and anode/hole transporting layer (hole injecting layer)/light emitting layer/hole barrier layer/electron transporting layer (electron injecting layer)/cathode.

In the organic EL device of the present invention, the light emitting layer preferably includes the polycyclic compound of the present invention as a host material. In addition, the light emitting layer preferably formed of a host material and a phosphorescent material, and the host material is preferably 40 the polycyclic compound.

In addition, the polycyclic compound of the present invention may be a host material used together with the phosphorescent material or an electron transporting material used together with the phosphorescent material. The triplet energy gap is preferably 2.2 to 3.2 eV and more preferably 2.5 to 3.2 eV.

As the phosphorescent material, a compound including iridium (Ir), osmium (Os), ruthenium (Ru), or platinum (Pt) is preferred from the viewpoints that the phosphorescent quantum efficiency is high and the external quantum efficiency of the device can be additionally improved. Metal complexes such as an iridium complex, an osmium complex, a ruthenium complex, and a platinum complex are more preferred. Of those, the iridium complex and the platinum complex are more preferred and an orthometalated iridium complex is most preferred. Specific examples of the metal complexes such as the iridium complex, the osmium complex, the ruthenium complex, and the platinum complex are described below.

[Chem 95] 45

In addition, the organic EL device of the present invention is preferably such that the light emitting layer contains a host material and a phosphorescent material, and contains a metal complex having a local maximum luminous wavelength of 500 nm or less

The organic EL device of the present invention preferably has a reductive dopant in an interfacial region between the cathode and an organic thin layer (for example, an electron injecting layer or a light emitting layer). Examples of the reductive dopant include at least one kind selected from an 30 alkali metal, an alkali metal complex, an alkali metal compound, an alkaline earth metal, an alkaline earth metal complex, an alkaline earth metal compound, a rare earth metal compound.

Preferred examples of the alkali metal include an alkali 35 metal having a work function of 2.9 eV or less, such as Na having a work function of 2.36 eV, K having a work function of 2.28 eV, Rb having a work function of 2.16 eV, and Cs having a work function of 1.95 eV. Of those, K, Rb, and Cs are more preferable, Rb or Cs is still more preferable, and Cs is 40 most preferable.

Preferred examples of the alkali earth metal include an alkali earth metal having a work function of 2.9 eV or less, such as Ca having a work function of 2.9 eV, Sr having a work function of 2.0 to 2.5 eV, and Ba having a work function of 45 2.52 eV.

Preferred examples of the rare earth metal include a rare earth metal having a work function of 2.9 eV or less, such as Sc, Y, Ce, Tb, and Yb.

Of those metals, a preferable metal has a particularly high 50 reductive ability, so improvement of light emission intensity and long life of organic EL device can be attained by adding a relatively small amount of the metal to an electron injecting region.

Examples of the alkali metal compound include an alkali 55 oxide such as Li₂O, Cs₂O, or K₂O, and an alkali halide such as LiF, NaF, CsF, or KF. Of those, LiF, Li₂O, or NaF is preferable.

Examples of the alkali earth metal compound include BaO, SrO, CaO, and mixtures thereof such as $Ba_mSr_{1-m}O$ (0<m<1) 60 and $Ba_mCa_{1-m}O$ (0<m<1). Of those, BaO, SrO, and CaO are preferable.

Examples of the rare earth metal compound include YbF₃, ScF₃, ScO₃, Y₂O₃, Ce₂O₃, GdF₃, and TbF₃. Of those, YbF₃, ScF₃, and TbF₃ are preferable.

The alkali metal complex, alkali earth metal complex, and rare earth metal complex are not particularly limited as long as they each include as a metal ion at least one of alkali metal ions, alkali earth metal ions, and rare earth metal ions. Meanwhile, preferable examples of a ligand include, but are not limited to, quinolinol, benzoquinolinol, acridinol, phenanthridinol, hydroxyphenyloxazole, hydroxyphenylthiazole, hydroxydiaryloxadiazole, hydroxydiarylthiadiazole, hydroxyphenylpyridine, hydroxyphenylbenzoimidazole, hydroxybenzotriazole, hydroxyfluborane, bipyridyl, phenanthroline, phthalocyanine, porphyrin, cyclopentadiene, β-diketones, azomethines, and derivatives thereof.

For the addition form of the reductive dopant, it is preferable that the reductive dopant be formed in a shape of a layer or an island in the interfacial region. A preferable example of the forming method includes a method in which an organic substance which is a light emitting material or an electron injecting material for forming the interfacial region is deposited at the same time as the reductive dopant is deposited by a resistant heating deposition method, thereby dispersing the reductive dopant in the organic substance. The disperse concentration by molar ratio of the organic compound to the reductive dopant is 100:1 to 1:100, and is preferably 5:1 to 1:5.

In a case where the reductive dopant is formed into the shape of a layer, the light emitting material or electron injecting material which serves as an organic layer in the interface is formed into the shape of a layer. After that, the reductive dopant is solely deposited by the resistant heating deposition method to form a layer preferably having a thickness of 0.1 to 15 nm.

In a case where the reductive dopant is formed into the shape of an island, the light emitting material or electron injecting material which serves as an organic layer in the interface is formed into the shape of an island. After that, the reductive dopant is solely deposited by the resistant heating deposition method to form an island preferably having a thickness of 0.05 to 1 nm.

When the organic EL device of the present invention has an electron injecting layer between the light emitting layer and the cathode, an electron transporting material to be used in the electron injecting layer is preferably an aromatic heterocyclic compound containing one or more heteroatoms in any one of its molecules, or particularly preferably a nitrogen-containing ring derivative.

The nitrogen-containing ring derivative is preferably, for example, a nitrogen-containing ring metal chelate complex represented by the following general formula (A).

[Chem 97]

$$R^{5}$$
 R^{5}
 R^{7}
 R^{4}
 R^{3}
 R^{2}
 R^{2}
 R^{2}
 R^{4}
 R^{3}
 R^{2}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{2}

 $R^2 \ {\rm to} \ R^7$ each independently represent a hydrogen atom, a halogen atom, an amino group, a hydrocarbon group each having 1 to 40 carbon atoms, an alkoxy group, an aryloxy group, an alkoxycarbonyl group, or a heterocyclic group, each of which may be substituted.

Examples of the halogen atom represented by R^2 to R^7 include a fluorine atom, a chlorine atom, a bromine atom, and an iodine atom.

Examples of the amino group that may be substituted and represented by R² to R⁷ include an alkylamino group, an arylamino group, and an aralkylamino group. Examples of the alkyl group in the alkylamino group include alkyl groups each having 1 to 40 carbon atoms such as a methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl 10 group, an s-butyl group, an isobutyl group, a t-butyl group, an n-pentyl group, an n-hexyl group, an n-heptyl group, an n-octyl group, an n-nonyl group, an n-decyl group, an n-undecyl group, an n-dodecyl group, an n-tridecyl group, an n-tetradecyl group, an n-pentadecyl group, an n-hexadecyl group, an n-heptadecyl group, an n-octadecyl group, an neopentyl group, a 1-methylpentyl group, a 2-methylpentyl group, a 1-pentylhexyl group, a 1-butylpentyl group, a 1-heptyloctyl group, a 3-methylpentyl group, a hydroxymethyl group, a 20 1-hydroxyethyl group, a 2-hydroxyethyl group, a 2-hydroxyisobutyl group, a 1,2-dihydroxyethyl group, a 1,3-dihydroxyisopropyl group, a 2,3-dihydroxy-t-butyl group, a 1,2,3-trihydroxypropyl group, a chloromethyl group, a 1-chloroethyl 25 group, a 2-chloroethyl group, a 2-chloroisobutyl group, a 1,2-dichloroethyl group, a 1,3-dichloroisopropyl group, a 2,3-dichloro-t-butyl group, a 1,2,3-trichloropropyl group, a bromomethyl group, a 1-bromoethyl group, a 2-bromoethyl group, a 2-bromoisobutyl group, a 1,2-dibromoethyl group, a $\,^{30}$ 1,3-dibromoisopropyl group, a 2,3-dibromo-t-butyl group, a 1,2,3-tribromopropyl group, a iodomethyl group, a 1-iodoethyl group, a 2-iodoethyl group, a 2-iodoisobutyl group, a 1,2-diiodoethyl group, a 1,3-diiodoisopropyl group, a 2,3diiodo-t-butyl group, a 1,2,3-triiodopropyl group, an aminomethyl group, a 1-aminoethyl group, a 2-aminoethyl group, a 2-aminoisobutyl group, a 1,2-diaminoethyl group, a 1,3-diaminoisopropyl group, a 2,3-diamino-t-butyl group, a 1,2,3-triaminopropyl group, a cyanomethyl group, a 1-cya-40 noethyl group, a 2-cyanoethyl group, a 2-cyanoisobutyl group, a 1,2-dicyanoethyl group, 1,3-dicyanoisopropyl group, a 2,3-dicyano-t-butyl group, a 1,2,3-tricyanopropyl group, a nitromethyl group, a 1-nitroethyl group, a 2-nitroethyl group, a 1,2-dinitroethyl group, a 2,3-dinitro-t-butyl group, and a 1,2,3-trinitropropyl group. Preferred are alkyl groups each having 1 to 20 carbon atoms and more preferred are alkyl groups each having 1 to 10 carbon atoms.

Examples of the aryl group in the arylamino group include 50 aryl groups each having 6 to 40 carbon atoms forming the aromatic ring such as a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, 4-phenanthryl group, a 55 9-phenanthryl group, a 1-naphthacenyl group, a 2-naphthacenyl group, a 9-naphthacenyl group, a 1-pyrenyl group, a 2-pyrenyl group, a 4-pyrenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, a p-terphenyl-2-yl group, an 60 m-terphenyl-4-yl group, a an m-terphenyl-3-yl group, an m-terphenyl-2-yl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl) phenyl group, a 3-methyl-2-naphthyl group, a 4-methyl-1naphthyl group, a 4-methyl-1-anthryl group, a 4'-methylbi- 65 phenylyl group, and a 4"-t-butyl-p-terphenyl-4-yl group. Preferred are aryl groups each having 6 to 20 carbon atoms

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forming the aromatic ring and more preferred are aryl groups each having 6 to 10 carbon atoms forming the aromatic ring.

Examples of the aralkyl group in the aralkylamino group include aralkyl groups each having 7 to 40 carbon atoms such as a benzyl group, a 1-phenylethyl group, a 2-phenylethyl group, a 1-phenylisopropyl group, a 2-phenylisopropyl group, a phenyl-t-butyl group, an α-naphthylmethyl group, a 1-α-naphthylethyl group, a 2-α-naphthylethyl group, a 1-αnaphthylisopropyl group, a 2-α-naphthylisopropyl group, a β-naphthylmethyl group, a 1-β-naphthylethyl group, a 2-βnaphthylethyl group, a 1-β-naphthylisopropyl group, a 2-βnaphthylisopropyl group, a 1-pyrrolylmethyl group, a 2-(1pyrrolyl)ethyl group, a p-methylbenzyl group, an m-methylbenzyl group, an o-methylbenzyl group, a p-chlorobenzyl group, an m-chlorobenzyl group, an o-chlorobenzyl group, a p-bromobenzyl group, an m-bromobenzyl group, an o-bromobenzyl group, a p-iodobenzyl group, an m-iodobenzyl group, an o-iodobenzyl group, a p-hydroxybenzyl group, an m-hydroxybenzyl group, an o-hydroxybenzyl group, a p-aminobenzyl group, an m-aminobenzyl group, an o-aminobenzyl group, a p-nitrobenzyl group, an m-nitrobenzyl group, an o-nitrobenzyl group, a p-cyanobenzyl group, an m-cyanobenzyl group, an o-cyanobenzyl group, a 1-hydroxy-2-phenylisopropyl group, and a 1-chloro-2-phenylisopropyl group. Preferred are aralkyl groups each having 7 to 20 carbon atoms and more preferred are aralkyl groups each having 7 to 10 carbon atoms.

Examples of the hydrocarbon groups each having 1 to 40 carbon atoms and represented by R² to R⁷ include substituted or unsubstituted alkyl groups, alkenyl groups, cycloalkyl groups, aryl groups, and aralkyl groups.

As the alkyl groups, the same examples of the alkyl groups in the above-mentioned alkylamino group are given, and alkyl groups each having 1 to 20 carbon atoms are preferred and alkyl groups each having 1 to 10 carbon atoms are more preferred.

Examples of the alkenyl group include alkenyl groups each having 2 to 40 carbon atoms such as a vinyl group, an allyl group, a 1-butenyl group, a 2-butenyl group, a 3-butenyl group, a 1,3-butanedienyl group, a 1-methylvinyl group, a styryl group, a 2,2-diphenylvinyl group, a 1,2-diphenylvinyl group, a 1-methylallyl group, a 2-methylallyl group, a 1-phenylallyl group, a 2-phenylallyl group, a 3-phenylallyl group, a 3,3-diphenylallyl group, a 1,2-dimethylallyl group, a 1,2-dimethylallyl group, a 3-phenyl-1-butenyl group, a 1-phenyl-1-butenyl group, and a 3-phenyl-1-butenyl group. Preferred are alkenyl groups each having 2 to 20 carbon atoms and more preferred are alkenyl groups each having 2 to 10 carbon atoms.

Examples of the cycloalkyl groups include cycloalkyl groups each having 3 to 40 carbon atoms forming the ring such as a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, a 4-methylcyclohexyl group, a 1-adamantyl group, a 2-adamantyl group, a 1-norbornyl group, and a 2-norbornyl group. Preferred are cycloalkyl groups each having 3 to 10 carbon atoms forming the ring are preferred.

As the aryl groups, the same examples of the aryl groups in the above-mentioned arylamino groups are given. Preferred are aryl groups each having 6 to 20 carbon atoms forming the aromatic ring and more preferred are aryl groups each having 6 to 10 carbon atoms forming the aromatic ring.

As the aralkyl groups, the same examples of the aralkyl groups in the above-mentioned aralkylamino groups are given. Preferred are aralkyl groups each having 7 to 20 carbon atoms and more preferred are aralkyl groups each having 7 to 10 carbon atoms.

As the alkoxy group that represented by R² to R⁷ and may be substituted, the same examples of the alkyl groups in the above-mentioned alkylamino groups are given as alkyl group moieties. Preferred are alkoxy groups each having 1 to 20 carbon atoms and more preferred alkoxy groups each having 5 1 to 10 carbon atoms.

As the aryloxy group that represented by R² to R⁷ and may be substituted, aryloxy groups each having the same aryl group in the above-mentioned arylamino group as an aryl $_{10}$ group moiety are given. Preferred are aryl groups each having 6 to 20 carbon atoms forming the aromatic ring and more preferred are aryl groups each having 6 to 10 carbon atoms forming the aromatic ring.

As the alkoxycarbonyl group that represented by R^2 to R^{7-15} and may be substituted, alkoxycarbonyl groups each having the same alkyl group in the above-mentioned alkylamino group as the alkyl group moiety are given. Preferred are alkoxycarbonyl groups each having 2 to 20 carbon atoms and more preferred are alkoxycarbonyl groups each having 2 to 10 carbon atoms.

The heterocyclic group that represented by R² to R⁷ and may be substituted is a monocycle or a fused ring. The heterocyclic group preferably has 1 to 20 carbon atoms forming $\,^{25}$ the aromatic ring, more preferably has 1 to 12 carbon atoms forming the aromatic ring, and still more preferably has 2 to 10 carbon atoms forming the aromatic ring. The heterocyclic group is an aromatic heterocyclic group having at least one 30 hetero atom selected form a nitrogen atom, an oxygen atom, a sulfur atom, and selenium atom. Examples of the heterocyclic group include groups derived from pyrrolidine, piperidine, piperazine, morpholine, thiophene, selenophene, furan, pyrrole, imidazole, pyrazole, pyridine, pyrazine, pyridazine, pyrimidine, triazole, triazine, indole, indazole, purine, thiazoline, thiazole, thiadiazole, oxazoline, oxazole, oxadiazole, quinoline, isoquinoline, phthalazine, naphthyridine, quinoxaline, quinazoline, cinnoline, pteridine, acridine, phenanthroline, phanazine, tetrazole, benzoimidazole, benzoxazole, benzothiazole, benzotriazole, tetrazaindene, carbazole, and azepine. Preferred are groups derived from furan, thiophene, pyridine, pyriazine, pyrimidine, pyridazine, triazine, quino- 45 exemplified compounds. line, phthalazine, naphthyridine, quinoxaline, and quinazoline, more preferred are groups derived from furan, thiophene, pyridine, and quinoline, and still more preferred is a quinolinyl group.

M represents aluminum (Al), gallium (Ga), or indium (In). Indium is preferred.

L⁴ in the formula (A) is a group represented by the following formula (A') or (A").

[Chem 98]

$$R^{8}$$
 R^{9}
 R^{10}
 R^{12}
 R^{11}
 R^{11}
 R^{10}

-continued

$$R^{14}$$
 R^{15}
 R^{16}
 R^{17}
 R^{18}
 R^{19}
 R^{20}
 R^{27}
 R^{23}
 R^{24}
 R^{25}

(In the formula, R⁸ to R¹² each independently represent a hydrogen atom, or a substituted or unsubstituted hydrocarbon group having 1 to 40 carbon atoms, and adjacent groups may form a cyclic structure. In addition, R13 to R27 each independently represent a hydrogen atom, or a substituted or unsubstituted hydrocarbon group having 1 to 40 carbon atoms, and adjacent groups may form a cyclic structure.)

As the hydrocarbon group having 1 to 40 carbon atoms and represented by R⁸ to R¹² in the formula (A') and R¹³ to R²⁷ in the formula (A"), the same specific examples of \mathbb{R}^2 to \mathbb{R}^7 are

In addition, examples of the divalent group in R⁸ to R¹² and R13 to R27 in the case where adjacent groups form a cyclic structure include a tetramethylene group, a pentamethylene group, a hexamethylene group, a diphenylmethane-2,2'-diyl group, a diphenylethane-3,3'-diyl group, and diphenylpropane-4,4'-diyl group.

Specific examples of the nitrogen-containing ring metal chelate complex represented by the formula (A) are shown below. However, the present invention is not limited to these

[Chem 99]

55

$$(A-1)$$

$$CH_3$$

$$CH_3$$

$$CH_3$$

$$CH_3$$

$$(A-2)$$

$$CH_3$$

$$\begin{array}{c} \begin{array}{c} \text{H}_3\text{C} \\ \\ \text{N} \end{array} \end{array}$$

$$\begin{array}{c} C_6H_5 \\ \\ C_6H_5 \\ \\ CH_3 \end{array}$$

(A-19)

(A-20)

-continued

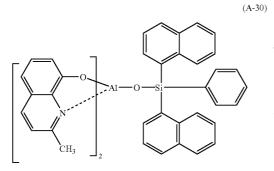
-continued

$$\begin{bmatrix} & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\$$

(A-24)

$$C_2H_5$$
 C_2H_3
 C_3H_3
 C

-continued



A nitrogen-containing heterocyclic derivative is a nitrogen-containing heterocyclic derivative composed of an organic compound having any one of the following general formulae, and a nitrogen-containing compound which is not a 55 metal complex is also an example of the derivative. Examples of the derivative include a five-or six-membered ring containing a skeleton represented by the following formula (a) and a derivative of a structure represented by the following formula

60

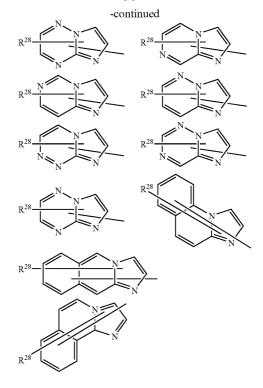
-continued



(In the formula (b), X represents a carbon atom or a nitrogen atom, and Z^1 and Z^2 each independently represent an atomic group capable of forming a nitrogen-containing heterocycle.)

An organic compound having a nitrogen-containing aromatic polycycle composed of a five-or six-membered ring is preferable. In the case of such nitrogen-containing aromatic polycycle having multiple nitrogen atoms, a nitrogen-containing aromatic polycyclic organic compound having a skeleton obtained by combining the above formulae (a) and (b) or the above formulae (a) and (c) is more preferable.

The nitrogen-containing group of the nitrogen-containing organic compound is selected from, for example, nitrogen-containing heterocyclic groups represented by the following 30 general formulae.



(In each of the formulae, R^{28} represents an aryl group having 6 to 40 carbon atoms, a heteroaryl group having 3 to 40 carbon atoms, an alkyl group having 1 to 20 carbon atoms, or an alkoxy group having 1 to 20 carbon atoms, n represents an integer of 0 to 5, and, when n represents an integer of 2 or more, multiple R^{28} s may be identical to or different from each other).

Further, a preferable specific compound is, for example, a nitrogen-containing heterocyclic derivative represented by the following formula.

$$HAr^a$$
- L^6 - Ar^b — Ar^c [Chem 105]

(In the formula, HAr^a represents a nitrogen-containing heterocycle which has 3 to 40 carbon atoms and may have a substituent, L^b represents a single bond, an arylene group which has 6 to 40 carbon atoms and may have a substituent, or a heteroarylene group which has 3 to 40 carbon atoms and may have a substituent, Ar^b represents a divalent aromatic hydrocarbon group which has 6 to 40 carbon atoms and may have a substituent, and Ar^c represents an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent.)

HAr^a is selected from, for example, the following group.

-continued

65

[Chem 107]

 Ar^c is selected from, for example, the following group.

-continued
$$R^{38}$$
 R^{39} Ar^d R^{42} R^{40}

(In the formulae, R²⁹ to R⁴² each independently represent a hydrogen atom, a halogen atom, an alkyl group having 1 to 20 carbon atoms, an alkoxy group having 1 to 20 carbon atoms, an aryloxy group having 6 to 40 carbon atoms, an aryl group which has 6 to 40 carbon atoms and may have a substituent, or
 a heteroaryl group having 3 to 40 carbon atoms, and Ar^d represents an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group having 3 to 40 carbon atoms.)

In addition, a nitrogen-containing heterocyclic derivative ²⁰ in which R²⁹ to R³⁶ in Ar^b represented by the above formula each represent a hydrogen atom is preferable.

In addition to the foregoing, the following compound (see JP 09-3448 A) is also suitably used.

25
$$R^{43}$$
 X^2 [Chem 110] R^{44} $N - R^{46}$ R^{45}

(In the formula, R⁴³ to R⁴⁶ each independently represent a hydrogen atom, a substituted or unsubstituted aliphatic group, a substituted or unsubstituted alicyclic group, a substituted or unsubstituted carbocyclic aromatic ring group, or a substituted or unsubstituted heterocyclic group, and X¹ and X² each independently represent an oxygen atom, a sulfur atom, or a dicyanomethylene group.)

In addition to the foregoing, the following compound (see JP 2000-173774 A) is also suitably used.

$$\begin{array}{c} \mathbb{R}^{47} \\ \mathbb{N} \\ \mathbb{C} = \mathbb{C} \\ \mathbb{C} \\ \mathbb{C} \\ \mathbb{C} \\ \mathbb{C} \\ \mathbb{C} \\ \mathbb{R}^{50} \end{array} \qquad \begin{bmatrix} \text{Chem 111} \\ \mathbb{R}^{49} \\ \mathbb{R}^{50} \\ \mathbb{R}^{50} \\ \mathbb{C} \\ \mathbb$$

 Ar^b is selected from, for example, the following ary lanthranil group.

In the formula, R⁴⁷, R⁴⁸, R⁴⁹, and R⁵⁰ represent groups identical to or different from one another, and each represent ⁵⁵ an aryl group represented by the following formula.

[Chem 109]

$$R^{30}$$
 R^{35}
 R^{35}
 R^{34}
 R^{34}
 R^{34}
 R^{34}
 R^{34}
 R^{35}
 R^{53}
 R^{54}

[Chem 109]

(In the formula, R⁵¹, R⁵², R⁵³, R⁵⁴, and R⁵⁵ represent groups identical to or different from one another, and each may represent a hydrogen atom, or at least one of them may represent a saturated or unsaturated alkoxyl, alkyl, amino, or alkylamino group.)

Further, a polymer compound containing the nitrogen-containing heterocyclic group or nitrogen-containing heterocyclic derivative is also permitted.

In addition, the electron transporting layer preferably contains at least one of the nitrogen-containing heterocyclic derivatives represented by the following general formulae (201) to (203).

[Chem 113]

$$\begin{array}{c}
N \\
N \\
N \\
R^{57}
\end{array}$$

$$\begin{array}{c}
L^{7} \\
Ar^{e} \\
- Ar^{f}
\end{array}$$
(201)

$$(202)$$

$$(R^{56})_n$$

$$L^7$$

$$Ar^g$$

In the formulae (201) to (203), R⁵⁶ represents a hydrogen atom, an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an 40 alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, n represents an integer of 0 to 4, R^{57} represents an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group having 1 to 20 carbon atoms, R⁵⁸ and R⁵⁹ each independently represent a hydrogen atom, an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group which has 1 to 20 carbon 55 atoms and may have a substituent, L⁷ represents a single bond, an arylene group which has 6 to 60 carbon atoms and may have a substituent, a pyridinylene group which may have a substituent, a quinolinylene group which may have a substituent, or a fluorenylene group which may have a substitu- 60 ent, Are represents an arylene group which has 6 to 60 carbon atoms and may have a substituent, a pyridinylene group which may have a substituent, or a quinolinylene group which may have a substituent, and Arf represents a hydrogen atom, an aryl group which has 6 to 60 carbon atoms and may have 65 a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group

which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group which has 1 to 20 carbon atoms and may have a substituent.

In the formulae, Ar^g represents an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, or a group represented by —Ar^e—Ar^f (Ar^e and Ar^f each have the same meaning as that described above).

It should be noted that, in the formulae (201) to (203), R⁵⁶ represents a hydrogen atom, an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group which has 1 to 20 carbon atoms and may have a substituent.

The aryl group which has 6 to 60 carbon atoms is prefer-20 ably an aryl group having 6 to 40 carbon atoms, or more preferably an aryl group having 6 to 20 carbon atoms, and specific examples of such groups include a phenyl group, a naphthyl group, an anthryl group, a phenanthryl group, a naphthacenyl group, a chrysenyl group, a pyrenyl group, a 25 biphenyl group, a terphenyl group, a tolyl group, a t-butylphenyl group, a (2-phenylpropyl)phenyl group, a fluoranthenyl group, a fluorenyl group, a monovalent group composed of spirobifluorene, a perfluorophenyl group, a perfluoronaphthyl group, a perfluoroanthryl group, a perfluorobiphenyl (203) 30 group, a monovalent group composed of 9-phenylanthracene, a monovalent group composed of 9-(1'-naphthyl) anthracene, a monovalent group composed of 9-(2'-naphthyl)anthracene, a monovalent group composed of 6-phenylchrysene, and a monovalent group composed of 9-[4-(diphenylamino) phe-35 nyl]anthracene; a phenyl group, a naphthyl group, a biphenyl group, a terphenyl group, a 9-(10-phenyl) anthryl group, a 9-[10-(1'-naphthyl)]anthryl group, a 9-[10-(2'-naphthyl)]anthryl group, or the like is preferable.

The alkyl group which has 1 to 20 carbon atoms is preferably an alkyl group having 1 to 6 carbon atoms, and specific examples of such group include a methyl group, an ethyl group, a propyl group, a butyl group, a pentyl group, a hexyl group, and a haloalkyl group such as a trifluoromethyl group. An alkyl group having 3 or more carbon atoms may be linear, cyclic, or branched.

The alkoxy group which has 1 to 20 carbon atoms is preferably an alkoxy group having 1 to 6 carbon atoms, and specific examples of such group include a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentyloxy group, and a hexyloxy group. An alkoxy group having 3 or more carbon atoms may be linear, cyclic, or branched.

Examples of the substituent of each group represented by R^{56} include a halogen atom, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, an aryloxy group which has 6 to 40 carbon atoms and may have a substituent, an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent.

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

Examples of the alkyl group which has 1 to 20 carbon atoms, the alkoxy group which has 1 to 20 carbon atoms, and the aryl group which has 6 to 40 carbon atoms include the same examples as those described above.

Examples of the aryloxy group which has 6 to 40 carbon atoms include a phenoxy group and a biphenyloxy group.

Examples of the heteroaryl group which has 3 to 40 carbon atoms include a pyrrolyl group, a furyl group, a thienyl group, a silolyl group, a pyridyl group, a quinolyl group, an isoquinolyl group, a benzofuryl group, an imidazolyl group, a pyrimidyl group, a carbazolyl group, a selenophenyl group, an oxadiazolyl group, and a triazolyl group.

n represents an integer of 0 to 4, or preferably 0 to 2.

In the formula (201), R^{57} represents an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl 10 group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group having 1 to 20 carbon atoms.

Specific examples of the respective groups, and preferable carbon numbers and preferable substituents of those groups are the same as those described for R.

In the formulae (202) and (203), R⁵⁸ and R⁵⁹ each independently represent a hydrogen atom, an aryl group which 20 has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group which has 1 to 20 carbon atoms and may have a substituent.

Specific examples of the respective groups, and preferable carbon numbers and preferable substituents of those groups are the same as those described for R⁵⁶.

In the formulae (201) to (203), L^7 represents a single bond, ³⁰ an arylene group which has 6 to 60 carbon atoms and may have a substituent, a pyridinylene group which may have a substituent, a quinolinylene group which may have a substituent, or a fluorenylene group which may have a substituent.

The arylene group which has 6 to 60 carbon atoms is preferably an arylene group having 6 to 40 carbon atoms, or more preferably an arylene group having 6 to 20 carbon atoms, and specific examples of such groups include divalent groups each formed by removing one hydrogen atom from the 40 aryl group described for R. Examples of the substituent of each group represented by $\rm L^7$ include the same examples as those described for $\rm R^{56}$.

In addition, L^7 preferably represents a group selected from the group consisting of the following groups.

In the formula (201), Are represents an arylene group which has 6 to 60 carbon atoms and may have a substituent, a pyridinylene group which may have a substituent, or a quinolinylene group which may have a substituent. Examples of the substituents of the respective groups represented by Ar^e and Ar^e include the same examples as those described for R⁵⁶.

In addition, Ar^e preferably represents any one of the groups selected from fused ring groups represented by the following formulae (101) to (110).

[Chem 115]

10

(108)

(109)

(111)

(112)

In the formulae (101) to (110), each fused ring may be bonded with a bonding group composed of a halogen atom, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, an aryloxy group which has 6 to 40 carbon atoms and may have a substituent, an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent, and, when multiple bonding groups of this kind are present, the bonding groups may be identical to or different from each other. Specific examples of the respective groups include the same examples as those described above.

In the formula (110), L' represents a single bond or a group selected from the group consisting of the following groups.

The formula (103) represented by ${\rm Ar}^e$ is preferably a fused 65 ring group represented by the following formulae (111) to (125).

(122)

-continued

-continued

In the formulae (111) to (125), each fused ring may be bonded with a bonding group composed of a halogen atom, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, an aryloxy group which has 6 to 40 carbon atoms and may have a substituent, an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent, and, when multiple bonding groups of this kind are present, the bonding groups may be identical to or different from each other. Specific examples of the respective groups include the same examples as those described above.

In the formula (201), Ar represents a hydrogen atom, an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, or an alkoxy group which has 1 to 20 carbon atoms and may have a substituent.

Specific examples of the respective groups, and preferable carbon numbers and preferable substituents of those groups are the same as those described for R^{56} .

In the formulae (202) and (203), Ar^g represents an aryl group which has 6 to 60 carbon atoms and may have a substituent, a pyridyl group which may have a substituent, a quinolyl group which may have a substituent, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, or a group represented by —Ar^e—Ar^f (Ar^e and Ar^f each have the same meaning as that described above).

10

Specific examples of the respective groups, and preferable carbon numbers and preferable substituents of those groups are the same as those described for R^{56} .

In addition, Arg preferably represents any one of the groups selected from fused ring groups represented by the following formulae (126) to (135).

[Chem 118]

-continued

In the formulae (126) to (135), each fused ring may be bonded with a bonding group composed of a halogen atom, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, an aryloxy group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent, and, when multiple bonding groups of this kind are present, the bonding groups may be identical to or different from each other. Specific examples of the respective groups include the same examples as those described above.

In the formula (135), L' is the same as that described above.

In the formulae (126) to (135), R' represents a hydrogen atom, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent. Specific examples of the respective groups include the same examples as those described above.

The general formula (128) represented by Ar^g is preferably a fused ring group represented by the following formulae (131) 40 (136) to (158).

45 [Chem 119]

(133) 55

(137)

-continued -continued

-continued

(151) R' (157)
20 (152) 25

(158) R'
(158) (153) 35

In the formulae (136) to (158), each fused ring may be bonded with a bonding group composed of a halogen atom, an alkyl group which has 1 to 20 carbon atoms and may have a substituent, an alkoxy group which has 1 to 20 carbon atoms and may have a substituent, an aryloxy group which has 6 to 40 carbon atoms and may have a substituent, an aryl group which has 6 to 40 carbon atoms and may have a substituent, or a heteroaryl group which has 3 to 40 carbon atoms and may have a substituent, and, when multiple bonding groups of this kind are present, the bonding groups may be identical to or different from each other. Specific examples of the respective groups include the same examples as those described above. R' is the same as that described above.

(155) 55 In addition, it is preferred that Ar and Ar each independently represent a group selected from the group consisting of the following groups.

Specific examples of the nitrogen-containing heterocyclic derivatives represented by the formulae (201) to (203) of the present invention are shown below. However, the present invention is not limited to these exemplified compounds.

It should be noted that HAr in the following tables represent any one of the following parts in the formulae (201) to (203).

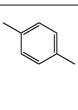
	HAr—L ⁷ —Ar ^e	—Ar ^f	
HAr	L^7	Ar^e	Ar^{f}

20

25

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[Chem 122]



	HAr—L ⁷ —Ar ^e —Ar ^f				
	HAr	L^7	Ar^e	Ar^f	
3	N N N				
4	N N				
5	N N N N N N N N N N N N N N N N N N N				
6	N N				
7	N N N N N N N N N N N N N N N N N N N				
8	N N				

HAr—L ⁷ —Ar ^e —Ar ^f				
	HAr	L ⁷	Ar^{e}	Arf
9	N N N N N N N N N N N N N N N N N N N			
10	N N N N N N N N N N N N N N N N N N N			
11	N N N N N N N N N N N N N N N N N N N			
12	N N			N
13	N N			
14	N N N N N N N N N N N N N N N N N N N			N

	-continued HAr—L ⁷ —Ar ^e —Ar ^f				
	HAr	L ⁷	Ar^e	Arf	
		[Chem 123]		
2-1	$H_{3}C$				
2	N N Et				
3	H ₃ C N				
4	H ₃ C N				
5	H ₃ C N				
6	CH ₃				

		-continued		
		HAr—L ⁷ —Ar ^e —	Arf	
	HAr	L^7	Ar^e	Arf
7				
8				
9				
		[Chem 124]		
3-1	N N N N N N N N N N N N N N N N N N N			
2	N N N N N N N N N N N N N N N N N N N			

		-continued		
		HAr — L^7 — Ar^e —	-Ar ^f	
	HAr	L^7	Ar^e	$\mathbf{A}_{\mathbf{r}^{\!f}}$
3	N N N N N N N N N N N N N N N N N N N			
4				
5	N N N N N N N N N N N N N N N N N N N			
6	N N N N N N N N N N N N N N N N N N N	[Chem 125]		
4-1	N	_		

		HAr — L^7 — Ar^e	—Ar ^f	
	HAr	L^7	Ar^e	Arf
2	N N			
3	N N			
4	N N	N N		
5	N N	N		
6	N N			
7				

		-continued	1	
		HAr — L^7 — Ar^e		
	HAr	L ⁷	Ar ^e	Arf
8	N N			
9	N N			
10	N N			
11	N N N N N N N N N N N N N N N N N N N			
12	N N N N N N N N N N N N N N N N N N N	[Chem 126]		
5-1	N N	[Circin 120]	CH ₃	

	389	.•	390	
		-contin		
	HAr	HAr—L ⁷ —A	Λr ^e —Ar ^r Ar ^e	\mathbf{Ar}^f
2	N N N N N N N N N N N N N N N N N N N			
3				
4			H ₃ C	I ₃
5				
6	N N N N N N N N N N N N N N N N N N N	[Chem 1	27)	
6-1		[Chem I		

-continued				
		HAr—L ⁷ —	Ar ^e —Ar ^f	
	HAr	Γ_{Δ}	Ar ^e	Ar
2				
3				
4				
5		[Chem	128]	
7-1		\	I	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \
, .T				

	-continued HAr—L ⁷ —Ar ^e —Ar ^f				
	HAr	L ⁷	Ar ^e	Ar	
2	N N N N N N N N N N N N N N N N N N N				
3					
4	N N				
5	N CH_3				
6	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$				
7	N CH_3				

	$HAr-L^7-Ar^e-Ar^f$					
	HAr	L^7	Are	Ar^{f}		
8	H ₃ C N					
9						
10	N CH_3					
8-1		[Chem 129		` ^		
0-1	N N					
2	N N					
3	N N N N N N N N N N N N N N N N N N N					

HAr—L ⁷ —Ar ^e —Ar ^f				
	HAr	L^7	Ar^e	Ar^f
4				
5	N N N N N N N N N N N N N N N N N N N			
6	N N N N N N N N N N N N N N N N N N N			
7	N N N N N N N N N N N N N N N N N N N			H
8	N N N N N N N N N N N N N N N N N N N			
9	N N N N N N N N N N N N N N N N N N N			

-continued				
		HAr—L ⁷ —Ar	e—Ar ^f	
	HAr	\mathbb{L}^7	Ar^{e}	Ar^f
10	N N N N N N N N N N N N N N N N N N N			
11	N N			H
12	N N			
13	N N N N N N N N N N N N N N N N N N N	[Chem 13		
9-1				
2				

HAr — L^7 — Ar^e — Ar^f				
	HAr	L ⁷	Ar^e	Ar
3	N N			
4	N N			
5	N N			
6				
7				
8	N N			
9	N N			

-continued				
		HAr—L ⁷ —Ar ^e	—Ar ^f	
	HAr	${ t L}^7$	Ar^e	Ar^f
10				
11	N N			
12				N
13	N N			
14		[Chem 131		
10-1	N CH ₃			
2	N Et			

HAr — L^7 — Ar^e — Ar^f			
HAr	L^7	Ar^c	\mathbf{Ar}^f
3 H ₃ C N			
4 H ₃ C N			
5 H ₃ C N			
6 CH ₃			
7 N			
8 N			

	-continued		
	HAr — L^7 — Ar^e —	Ar^f	
HAr	L^7	Ar^e	Ar
9			
	[Chem 132]		
11-1 N			
3 N N N N N N N N N N N N N N N N N N N			
4 N N N			
5 N N N			
6 N			

	$HAr-L^7-Ar^e-Ar^f$			
	HAr	L ⁷	Ar^e	Ar
		[Chem 133]]	
12-1				
2				
3	N N			
4	N N	N		
5	N N	N		
6				
7				

	HAr—L ⁷ —Ar ^e —Ar ^f				
	НАг	L^7	Ar^e	Ar ^f	
8	N				
9	N N				
10	N				
11	N N	[Chem 1	34]		
13-1	N		CH ₃		
2	N N				
3					

	-continued				
		HAr—L ⁷ —	-Ar ^e —Ar ^f		
	HAr	L^7	Ar^e	Arf	
4			H ³ CC CH ³		
5					
6	N	[Chem	135]		
14-1	N N				
2					
3	N N				
4	N N				

			anued	
	НАг	$\frac{\text{HAr}\text{L}^7}{\text{L}^7}$	—Ar ^e —Ar ^f Ar ^e	Ar
5	N N	[Cher	n 136]	
15-1		\		
2	\	_		
3	/	_		
4	N.	_		
5		_		
	$_{ m CH_3}$			

	-continued				
-		$HAr-L^7-Ar^e$	-Ar ^f		
	HAr	L^7	Ar^e	Ar	
6	H ₃ C				
7	N CH ₃				
8	$H_{3}C$				
9	N N				
10	N CH_3	(Cham 127)			
16-1	N N N N N N N N N N N N N N N N N N N	[Chem 137]			

	HAr—L ⁷ —Ar ^e —Ar ^f			
	HAr	L^7	Ar^e	Ar ^f
2	N N N N N N N N N N N N N N N N N N N			
3				
4	N N			
5				
6	N N N N N N N N N N N N N N N N N N N			
7	H_3C CH_3			

$HAr_L^7_Ar^e_Ar^r$							
	HAr	L ⁷	Ar ^e	Arf			
8	H_3C CH_3						
		[Chem 138]					
17-1							
2	N N N N N N N N N N N N N N N N N N N						
3							
4	N N N N N N N N N N N N N N N N N N N						

HAr—L ⁷ —Ar ^e —Ar ^f						
	HAr	L^7	Ar ^e	Ar		
5	N N N N N N N N N N N N N N N N N N N					
6						
7						
8	N N N					

Of those specific examples, (1-1), (1-5), (1-7), (2-1), (3-1), (4-2), (4-6), (7-2), (7-7), (7-8), (7-9), (9-1), and (9-7) are particularly preferred.

In addition, as the nitrogen-containing ring derivative, nitrogen-containing five-membered ring derivative are also preferably exemplified. Examples of the nitrogen-containing five-membered ring include an imidazole ring, a triazole ring, a tetrazole ring, an oxadiazole ring, a thiadiazole ring, an oxatriazole ring, and a thiatriazole ring. Examples of the nitrogen-containing five-membered ring derivative include a benzoimidazole ring, a benzotriazole ring, a pyridinoimidazole ring, a pyrimidinoimidazole ring, and a pyridazinoimidazole ring. Particularly preferred is the compound represented by the following general formula (B).

[Chem 139]

$$L^{B} \xrightarrow{X} Z^{B2}$$

$$X^{B2} \xrightarrow{X} n_{B2}$$
(B)

In the general formula (B), L^B represents a divalent or more bonding group. Examples thereof include a carbon atom, a silicon atom, a nitrogen atom, a boron atom, an oxygen atom, a sulfur atom, metal atoms (for example, a barium atom, a beryllium atom), aromatic hydrocarbon rings, and aromatic heterocycles. Of those, preferred are a carbon atom, a nitro-

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35

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gen atom, a silicon atom, a boron atom, an oxygen atom, a sulfur atom, aromatic hydrocarbon rings, and aromatic heterocyclic groups, and more preferred are a carbon atom, a silicon atom, aromatic hydrocarbon rings, and aromatic heterocyclic groups.

The aromatic hydrocarbon rings and aromatic heterocyclic groups represented by L^B may have a substituent. Examples of the substituent include alkyl groups, alkenyl groups, aryl groups, amino groups, alkoxy groups, aryloxy groups, acyl 10 groups, alkoxycarbonyl groups, aryloxycarbonyl groups, acyloxy groups, acylamino groups, alkoxycarbonylamino groups, aryloxycarbonylamino groups, sulfonylamino groups, sulfamoyl groups, carbamoyl groups, alkylthio 15 groups, arylthio groups, sulfonyl groups, halogen atoms, cyano groups, and aromatic heterocyclic groups. Preferred are alkyl groups, aryl groups, alkoxy groups, aryloxy groups, halogen atoms, cyano groups, and aromatic heterocyclic groups, more preferred are alkyl groups, aryl groups, alkoxy $\,^{20}$ groups, aryloxy groups, and aromatic heterocyclic groups, and particularly preferred are alkyl groups, aryl groups, alkoxy groups, and aromatic heterocyclic groups.

Specific examples of L^B include compounds represented ²⁵ below

ĊH₂

 X^{B2} in the general formula (B) represents —O—, —S—, or —N(R^{B2})—. R^{B2} represents a hydrogen atom, an aliphatic hydrocarbon group, an aryl group, or a heterocyclic group.

The aliphatic hydrocarbon group represented by R^{B2} is a linear or branched alkyl group (having preferably 1 to 20, more preferably 1 to 12, or particularly preferably 1 to 8 carbon atoms such as a methyl group, an ethyl group, an n-decyl group, or an n-hexadecyl group), a cycloalkyl group (having preferably 3 to 10 carbon atoms forming the ring such as a cyclopropyl group, a cyclopentyl group, or a cyclohexyl group), an alkenyl group (having preferably 2 to 20, more preferably 2 to 12, or particularly preferably 2 to 8 carbon atoms such as a vinyl group, an alkynyl group (having preferably 2 to 20, more preferably 2 to 12, or particularly preferably 2 to 20, more preferably 2 to 12, or particularly preferably 2 to 8 carbon atoms such as a propargyl group or a 3-pentynyl group), or is preferably an alkyl group.

The aryl group represented by R^{B2} is a monocycle or a fused ring, and is an aryl group having preferably 6 to 30, more preferably 6 to 20, or still more preferably 6 to 12 carbon atoms forming the ring. Examples of such groups include a phenyl group, a 2-methylphenyl group, a 3-methylphenyl group, a 4-methylphenyl group, a 2-methoxyphenyl group, a

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3-trifluoromethylphenyl group, a pentafluorophenyl group, a 1-naphthyl group, and a 2-naphthyl group. Of those, a phenyl group or a 2-methylphenyl group is preferable.

The heterocyclic group represented by R^{B2} is a monocycle or a fused ring, and is a heterocyclic group having preferably 1 to 20, more preferably 1 to 12, or still more preferably 2 to 10 carbon atoms forming the aromatic ring. The heterocyclic group is an aromatic heterocyclic group containing at least one heteroatom selected from a nitrogen atom, an oxygen atom, a sulfur atom, and a selenium atom. Examples of the heterocyclic group include groups derived from pyrrolidine. piperidine, piperazine, morpholine, thiophene, selenophene, furan, pyrrole, imidazole, pyrazole, pyridine, pyrazine, pyridazine, pyrimidine, triazole, triazine, indole, indazole, purine, thiazoline, thiazole, thiadiazole, oxazoline, oxazole, oxadiazole, quinoline, isoquinoline, phthalazine, naphthyridine, quinoxaline, quinazoline, cinnoline, pteridine, acridine, phenanthroline, phanazine, tetrazole, benzoimidazole, benzoxazole, benzothiazole, benzotriazole, tetrazaindene, carbazole, azepine, and the like. Preferred are groups derived from 20 furan, thiophene, pyridine, pyrazine, pyrimidine, pyridazine, triazine, quinoline, phthalazine, naphthyridine, quinoxaline, and quinazoline, more preferred are groups derived from furan, thiophene, pyridine, and quinoline, and still more preferred is a quinolinyl group.

The aliphatic hydrocarbon group, the aryl group, and the heterocyclic group each represented by $R^{\mathcal{B}^2}$ may each have a substituent, and the substituent is preferably an alkyl group, an alkenyl group, an alkynyl group, an aryl group, an amino group, an alkoxy group, an aryloxy group, an acyl group, an alkoxycarbonyl group, an aryloxycarbonyl group, an acyloxy group, an acylamino group, an alkoxycarbonylamino group, an aryloxycarbonylamino group, a sulfonylamino group, a sulfamoyl group, a carbamoyl group, an alkylthio group, an arylthio group, a sulfonyl group, a halogen atom, a cyano group, or an aromatic heterocyclic group, more preferably an 35 alkyl group, an aryl group, an alkoxy group, an aryloxy group, a halogen atom, a cyano group, or an aromatic heterocyclic group, still more preferably an alkyl group, an aryl group, an alkoxy group, an aryloxy group, or an aromatic heterocyclic group, or particularly preferably an alkyl group, an aryl 40 group, an alkoxy group, or an aromatic heterocyclic group.

R⁸² preferably represents an aliphatic hydrocarbon group,

R⁸² preferably represents an aliphatic hydrocarbon group, an aryl group, or a heterocyclic group, more preferably represents an aliphatic hydrocarbon group (having preferably 6 to 30, more preferably 6 to 20, or still more preferably 6 to 12 carbon atoms) or an aryl group, or still more preferably represents an aliphatic hydrocarbon group (having preferably 1 to 20, more preferably 1 to 12, or still more preferably 2 to 10 carbon atoms).

 X^{B2} preferably represents —O— or —N(R^{B2})—, or more 50 preferably represents —N(R^{B2})—.

 Z^{B2} represents atoms necessary for forming an aromatic ring. The aromatic ring formed of Z^{B2} is any one of aromatic hydrocarbon rings and aromatic heterocyclic rings. Specific examples thereof include a benzene ring, a pyridine ring, a pyrazine ring, a pyrimidine ring, a pyridazine ring, a triazine ring, a pyrrole ring, a furan ring, a thiophene ring, a selenophene ring, a tellurophene ring, an imidazole ring, a thiazole ring, a selenazole ring, a tellulazole ring, a thiadiazole ring, an oxadiazole ring, and a pyrazole ring. Preferred are a benzene ring, a pyridine ring, and a pyridazine ring, a pyridine ring, and particularly preferred is a pyridine ring.

The aromatic ring formed of Z^{B2} may further form a fused 65 ring with any other rings, or may have a substituent. Examples of the substituent include the same examples as those

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described for the substituent of the group represented by L^B . and the substituent is preferably an alkyl group, an alkenyl group, an alkynyl group, an aryl group, an amino group, an alkoxy group, an aryloxy group, an acyl group, an alkoxycarbonyl group, an aryloxycarbonyl group, an acyloxy group, an acylamino group, an alkoxycarbonylamino group, an aryloxycarbonylamino group, a sulfonylamino group, a sulfamoyl group, a carbamoyl group, an alkylthio group, an arylthio group, a sulfonyl group, a halogen atom, a cyano group, or a heterocyclic group, more preferably an alkyl group, an aryl group, an alkoxy group, an aryloxy group, a halogen atom, a cyano group, or a heterocyclic group, still more preferably an alkyl group, an aryl group, an alkoxy group, an aryloxy group, or an aromatic heterocyclic group, or particularly preferably an alkyl group, an aryl group, an alkoxy group, or an aromatic heterocyclic group.

 n^{B2} represents an integer of 1 to 4, or preferably 2 or 3.

Of the nitrogen-containing five-membered ring derivatives each represented by the general formula (B), a derivative represented by the following general formula (B') is more preferable.

In the general formula (B'), R^{B71} , R^{B72} , and R^{B73} each have the same meaning as that of R^{B2} in the general formula (B), and the preferable ranges of R^{B71} , R^{B72} , and R^{B73} are also the same as those of R^{B2} .

In the formula, Z^{B71} , Z^{B72} and Z^{B73} each have the same meaning as that of Z^{B2} in the general formula (B), and the preferable ranges of Z^{B71} , Z^{B72} , and Z^{B73} are also the same as those of Z^{B2} .

In the formula, \mathcal{L}^{B71} , \mathcal{L}^{B72} , and \mathcal{L}^{B73} each represent a linking group, and examples of the linking group include examples obtained by making the examples of \mathcal{L}^B in the general formula (B) divalent. The linking group is preferably a single bond, a divalent aromatic hydrocarbon ring group, or a linking group composed of a combination of two or more of them, or is more preferably a single bond. \mathcal{L}^{B71} , \mathcal{L}^{B72} , and \mathcal{L}^{B73} may each have a substituent. Examples of the substituent include the same examples as those described for the substituent of the group represented by \mathcal{L}^B in the general formula (B), and preferable examples as those described for the substituent of the group represented by \mathcal{L}^B in the general formula (B).

In the formula, Y^B represents a nitrogen atom, a 1,3,5-benzenetriyl group, or a 2,4,6-triazinetriyl group. The 1,3,5-benzenetriyl group may have a substituent at any one of its 2-, 4-, and 6-positions, and examples of the substituent include an alkyl group, an aromatic hydrocarbon ring group, and a halogen atom.

Specific examples of the nitrogen-containing five-membered ring derivative represented by the general formula (B)

or (B^\prime) are shown below. However, the present invention is not limited to these exemplified compounds.

$$\begin{array}{c} (B-3) \\ H_3C \\ N \\ N \\ CH_3 \end{array}$$

$$\begin{array}{c} H_3C \\ H_3C \\ \end{array}$$

-continued

-continued

[Chem 143]

$$(B-13)$$

$$N$$

$$N$$

$$CH_3$$

$$N$$

$$N$$

15

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-continued

A compound of which each of the electron injecting layer 40 and the electron transporting layer is constituted is, for example, a compound having a structure obtained by combining an electron-deficient, nitrogen-containing five-membered ring skeleton or electron-deficient, nitrogen-containing 45 six-membered ring skeleton and a substituted or unsubstituted indole skeleton, substituted or unsubstituted carbazole skeleton, or substituted or unsubstituted azacarbazole skeleton as well as the polycyclic compound of the present inven- $_{\rm 50}$ tion. In addition, a suitable electron-deficient, nitrogen-containing five-membered ring skeleton or electron-deficient, nitrogen-containing six-membered ring skeleton is a molecular skeleton such as a pyridine, pyrimidine, pyrazine, triazine, triazole, oxadiazole, pyrazole, imidazole, quinoxaline, or $^{\,55}$ pyrrole skeleton, or benzimidazole or imidazopyridine obtained when two or more of them fuse with each other. Of those combinations, a preferable combination is, for example, a combination of a pyridine, pyrimidine, pyrazine, or triazine 60 skeleton and a carbazole, indole, azacarbazole, or quinoxaline skeleton. The above-mentioned skeleton may be substituted or unsubstituted.

Specific examples of an electron transportable compound $_{65}$ are shown below. However, the present invention is not particularly limited to these examples.

-continued

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Each of the electron injecting layer and the electron transporting layer may be of a monolayer structure composed of one or two or more kinds of the above materials, or may be of a multi-layered structure composed of multiple layers identical to or different from each other in composition. Materials for those layers each preferably have a π -electron-deficient, nitrogen-containing heterocyclic group.

In addition, an insulator or semiconductor serving as an inorganic compound as well as the nitrogen-containing ring derivative is preferably used as a component of the electron injecting layer. When the electron injecting layer is constituted of an insulator or semiconductor, current leakage can be effectively prevented, and the electron injecting property of the layer can be improved.

As the insulator, at least one metal compound selected from the group consisting of alkali metal chalcogenides, alkaline earth metal chalcogenides, alkali metal halides, and alkaline earth metal halides is preferably used. It is preferable that the electron injecting layer be composed of the above-mentioned substance such as the alkali metal chalcogenide since the electron injecting property can be further improved. To be specific, preferable examples of the alkali metal chalcogenide include Li₂O, K₂O, Na₂S, Na₂Se, and Na₂O, and preferable examples of the alkaline earth metal chalcogenide include CaO, BaO, SrO, BeO, BaS, and CaSe. Preferable examples of the alkali metal halide include LiF, NaF, KF, LiCl, KCl, and NaCl. Preferable examples of the alkaline earth metal halide include fluorides such as CaF₂, BaF₂, SrF₂, MgF₂, and BeF₂ and halides other than the fluorides.

In addition, examples of the semiconductor include oxides, 60 nitrides, and oxide nitrides containing at least one element selected from the group consisting of Ba, Ca, Sr, Yb, Al, Ga, In, Li, Na, Cd, Mg, Si, Ta, Sb, and Zn, and they may be used alone or in combination of two or more. It is preferable that the inorganic compound composing the electron injecting 65 layer form a crystallite or amorphous insulating thin film. When the electron injecting layer is composed of the insulat-

ing thin film described above, a more uniform thin film can be formed, and defects of pixels such as dark spots can be decreased. Examples of the inorganic compound include alkali metal chalcogenides, alkaline earth metal chalcogenides, alkali metal halides.

In addition, the above-mentioned reducing dopant can be preferably incorporated into the electron injecting layer in the present invention.

It should be noted that the thickness of each of the electron injecting layer and the electron transporting layer, which is not particularly limited, is preferably 1 to 100 nm.

An aromatic amine compound such as an aromatic amine derivative represented by a general formula (I) is suitably used in the hole injecting layer or hole transporting layer (a hole injecting/transporting layer is also included in this category).

[Chem 146]
$$\begin{array}{c}
Ar^{1} & Ar^{3} \\
N - L - N & 4
\end{array}$$
(I)

In the general formula (I), Ar¹ to Ar⁴ each represent a substituted or unsubstituted aryl group having 6 to 50 carbon atoms forming the aromatic ring, or a substituted or unsubstituted heteroaryl group having 5 to 50 atoms forming the aromatic ring.

Examples of the substituted or unsubstituted aryl group having 6 to 50 carbon atoms forming the aromatic ring include a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, a 4-phenanthryl group, a 9-phenanthryl group, a 1-naphthacenyl group, a 2-naphthacenyl group, a 9-naphthacenyl group, a 1-pyrenyl group, a 2-pyrenyl group, a 4-pyrenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, a p-terphenyl-2-yl group, an m-terphenyl-4-yl group, an m-terphenyl-3-yl group, an m-terphenyl-2-yl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl)phenyl group, a 3-methyl-2-naphthyl group, a 4-methyl-1-naphthyl group, a 4-methyl-1-anthryl group, a 4'-methylbiphenylyl group, a 4"-t-butyl-p-terphenyl-4-yl group, a fluoranthenyl group, and a fluorenyl group.

Examples of the substituted or unsubstituted heteroaryl group having 5 to 50 atoms forming the aromatic ring include a 1-pyrrolyl group, a 2-pyrrolyl group, a 3-pyrrolyl group, a pyrazinyl group, a 2-pyridinyl group, a 3-pyridinyl group, a 4-pyridinyl group, a 1-indolyl group, a 2-indolyl group, a 3-indolyl group, a 4-indolyl group, a 5-indolyl group, a 6-indolyl group, a 7-indolyl group, a 1-isoindolyl group, a 2-isoindolyl group, a 3-isoindolyl group, a 4-isoindolyl group, a 5-isoindolyl group, a 6-isoindolyl group, a 7-isoindolyl group, a 2-furyl group, a 3-furyl group, a 2-benzofuranyl group, a 3-benzofuranyl group, a 4-benzofuranyl group, a 5-benzofuranyl group, a 6-benzofuranyl group, a 7-benzofuranyl group, a 1-isobenzofuranyl group, a 3-isobenzofuranyl group, a 4-isobenzofuranyl group, a 5-isobenzofuranyl group, a 6-isobenzofuranyl group, a 7-isobenzofuranyl group, a quinolyl group, a 3-quinolyl group, a 4-quinolyl group, a 5-quinolyl group, a 6-quinolyl group, a 7-quinolyl group, an 8-quinolyl group, a 1-isoquinolyl group, a 3-iso-

quinolyl group, a 4-isoquinolyl group, a 5-isoquinolyl group, a 6-isoquinolyl group, a 7-isoquinolyl group, an 8-isoquinolyl group, a 2-quinoxalinyl group, a 5-quinoxalinyl group, a 6-quinoxalinyl group, a 1-carbazolyl group, a 2-carbazolyl group, a 3-carbazolyl group, a 4-carbazolyl group, a 9-carbazolyl group, a 1-phenanthridinyl group, a 2-phenanthridinyl group, a 3-phenanthridinyl group, a 4-phenanthridinyl group, a 6-phenanthridinyl group, a 7-phenanthridinyl group, an 8-phenanthridinyl group, a 9-phenanthridinyl group, a 10-phenanthridinyl group, a 1-acridinyl group, a 10 2-acridinyl group, a 3-acridinyl group, a 4-acridinyl group, a 9-acridinyl group, a 1,7-phenanthrolin-2-yl group, a 1,7phenanthrolin-3-yl group, a 1,7-phenanthrolin-4-yl group, a 1,7-phenanthrolin-5-yl group, a 1,7-phenanthrolin-6-yl group, a 1,7-phenanthrolin-8-yl group, a 1,7-phenanthrolin- 15 9-yl group, a 1,7-phenanthrolin-10-yl group, a 1,8-phenanthrolin-2-yl group, a 1,8-phenanthrolin-3-yl group, a 1,8phenanthrolin-4-yl group, a 1,8-phenanthrolin-5-yl group, a 1,8-phenanthrolin-6-yl group, a 1,8-phenanthrolin-7-yl group, a 1,8-phenanthrolin-9-yl group, a 1,8-phenanthrolin- 20 10-yl group, a 1,9-phenanthrolin-2-yl group, a 1,9-phenanthrolin-3-yl group, a 1,9-phenanthrolin-4-yl group, a 1,9phenanthrolin-5-yl group, a 1,9-phenanthrolin-6-yl group, a 1,9-phenanthrolin-7-yl group, a 1,9-phenanthrolin-8-yl group, a 1,9-phenanthrolin-10-yl group, a 1,10-phenanthro- 25 lin-2-yl group, a 1,10-phenanthrolin-3-yl group, a 1,10phenanthrolin-4-yl group, a 1,10-phenanthrolin-5-yl group, a 2,9-phenanthrolin-1-yl group, a 2,9-phenanthrolin-3-yl group, a 2,9-phenanthrolin-4-yl group, a 2,9-phenanthrolin-5-yl group, a 2,9-phenanthrolin-6-yl group, a 2,9-phenan- 30 throlin-7-yl group, a 2,9-phenanthrolin-8-yl group, a 2,9phenanthrolin-10-yl group, a 2,8-phenanthrolin-1-yl group, a 2,8-phenanthrolin-3-yl group, a 2,8-phenanthrolin-4-yl group, a 2,8-phenanthrolin-5-yl group, a 2,8-phenanthrolin-6-yl group, a 2,8-phenanthrolin-7-yl group, a 2,8-phenan- 35 throlin-9-yl group, a 2,8-phenanthrolin-10-yl group, a 2,7phenanthrolin-1-yl group, a 2,7-phenanthrolin-3-yl group, a 2,7-phenanthrolin-4-yl group, a 2,7-phenanthrolin-5-yl group, a 2,7-phenanthrolin-6-yl group, a 2,7-phenanthrolin-8-yl group, a 2,7-phenanthrolin-9-yl group, a 2,7-phenan- 40 throlin-10-yl group, a 1-phenazinyl group, a 2-phenazinyl group, a 1-phenothiazinyl group, a 2-phenothiazinyl group, a 3-phenothiazinyl group, a 4-phenothiazinyl group, a 10-phenothiazinyl group, a 1-phenoxazinyl group, a 2-phenoxazinyl group, a 3-phenoxazinyl group, a 4-phenoxazinyl group, a 45 10-phenoxazinyl group, a 2-oxazolyl group, a 4-oxazolyl group, a 5-oxazolyl group, a 2-oxadiazolyl group, a 5-oxadiazolyl group, a 3-furazanyl group, a 2-thienyl group, a 3-thienyl group, a 2-methylpyrrol-1-yl group, a 2-methylpyrrol-3-yl group, a 2-methylpyrrol-4-yl group, a 2-methylpyr- 50 rol-5-yl group, a 3-methylpyrrol-1-yl group, a 3-methylpyrgroup, a 3-methylpyrrol-4-yl 3-methylpyrrol-5-yl group, a 2-t-butylpyrrol-4-yl group, a 3-(2-phenylpropyl)pyrrol-1-yl group, a 2-methyl-1-indolyl group, a 4-methyl-1-indolyl group, a 2-methyl-3-indolyl 55 group, a 4-methyl-3-indolyl group, a 2-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 2-t-butyl3-indolyl group, and a 4-t-butyl3-indolyl group. Preferred are a phenyl group, a naphthyl group, a biphenyl group, an anthranyl group, a phenanthryl group, a pyrenyl group, a chrycenyl group, a 60 fluoranthenyl group, and a fluorenyl group.

L represents a linking group, and specifically, a substituted or unsubstituted arylene group having 6 to 50 carbon atoms forming the aromatic ring, a substituted or unsubstituted heteroarylene group having 5 to 50 atoms forming the aromatic 65 ring, or a divalent group in which two or more arylene groups or heteroarylene groups are bonded by a single bond, an ether

bond, a thioether bond, with an alkylene group having 1 to 20 carbon atoms, an alkenylene group having 2 to 20 carbon atoms, and an amino group. Examples of the arylene group having 6 to 50 carbon atoms forming the aromatic ring include a 1,4-phenylene group, a 1,2-phenylene group, a 1,3phenylene group, a 1,4-naphthylene group, a 2,6-naphthylene group, a 1,5-naphthylene group, a 9,10-anthranylene group, a 9,10-phenanthrenylene group, a 3,6-phenanthrenylene group, 1,6-pyrenylene group, a 2,7-pyrenylene group, a 6,12chrycenylene group, a 4,4'-biphenylene group, a 3,3'-biphenylene group, a 2,2-biphenylene group, and a 2,7-fluorenylene group. Examples of the arylene group having 5 to 50 atoms forming the aromatic ring include a 2,5-thiophenylene group, a 2,5-silolylene group, and a 2,5-oxadiazolylene group. Preferred are a 1,4-phenylene group, a 1,2-phenylene group, a 1,3-phenylene group, a 1,4-naphthylene group, a 9,10-anthranylene group, a 6,12-chrysenylene group, a 4,4'biphenylene group, a 3,3'-biphenlene group, a 2,2'-biphenylene group, and a 2,7-fluorenylene group.

In the case where L represents a linking group formed of two or more arylene groups or heteroarylene groups, adjacent arylene groups or heteroarylene groups may be bonded to each other through a divalent group to form a ring. Examples of the divalent group forming a ring include a tetramethylene group, a pentamethylene group, a hexamethylene group, a diphenylmethane-2,2'-diyl group, a diphenyl ethane-3,3'-diyl group, and a diphenylpropane-4,4'-diyl group.

The substituent of each of Ar¹ to Ar⁴ and L is, for example, a substituted or unsubstituted aryl group having 6 to 50 carbon atoms forming the aromatic ring, a substituted or unsubstituted heteroaryl group having 5 to 50 atoms forming the aromatic ring, a substituted or unsubstituted alkyl group having 1 to 50 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 50 carbon atoms, a substituted or unsubstituted alkoxy group having 1 to 50 carbon atoms, a substituted or unsubstituted aralkyl group having 7 to 50 carbon atoms, a substituted or unsubstituted aryloxy group having 6 to 50 carbon atoms forming the aromatic ring, a substituted or unsubstituted heteroaryloxy group having 5 to 50 atoms forming the aromatic ring, a substituted or unsubstituted arylthio group having 6 to 50 carbon atoms forming the aromatic ring, a substituted or unsubstituted heteroarylthio group having 5 to 50 atoms forming the aromatic ring, a substituted or unsubstituted alkoxycarbonyl group having 2 to 50 carbon atoms, an amino group substituted by a substituted or unsubstituted aryl group having 6 to 50 carbon atoms forming the aromatic ring or by a substituted or unsubstituted heteroaryl group having 5 to 50 atoms forming the aromatic ring, a halogen group, a cyano group, a nitro group, or a hydroxyl group.

Examples of the substituted or unsubstituted aryl group having 6 to 50 carbon atoms forming the aromatic ring include a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, a 4-phenanthryl group, a 9-phenanthryl group, a 1-naphthacenyl group, a 2-naphthacenyl group, a 9-naphthacenyl group, a 2-pyrenyl group, a 4-pyrenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, an m-terphenyl-4-yl group, an m-terphenyl-2-yl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl)phenyl group, a 3-methyl-2-naphthyl group, a 4-methyl-1-naphthyl

group, a 4-methyl-1-anthryl group, a 4'-methylbiphenylyl group, a 4"-t-butyl-p-terphenyl-4-yl group, a fluoranthenyl group, and a fluorenyl group.

Examples of the substituted or unsubstituted heteroaryl group having 5 to 50 atoms forming the aromatic ring include a 1-pyrrolyl group, a 2-pyrrolyl group, a 3-pyrrolyl group, a pyrazinyl group, a 2-pyridinyl group, a 3-pyridinyl group, a 4-pyridinyl group, a 1-indolyl group, a 2-indolyl group, a 3-indolyl group, a 4-indolyl group, a 5-indolyl group, a 6-indolyl group, a 7-indolyl group, a 1-isoindolyl group, a 10 2-isoindolyl group, a 3-isoindolyl group, a 4-isoindolyl group, a 5-isoindolyl group, a 6-isoindolyl group, a 7-isoindolyl group, a 2-furyl group, a 3-furyl group, a 2-benzofuranyl group, a 3-benzofuranyl group, a 4-benzofuranyl group, a 5-benzofuranyl group, a 6-benzofuranyl group, a 7-benzo- 15 furanyl group, a 1-isobenzofuranyl group, a 3-isobenzofuranyl group, a 4-isobenzofuranyl group, a 5-isobenzofuranyl group, a 6-isobenzofuranyl group, a 7-isobenzofuranyl group, a quinolyl group, a 3-quinolyl group, a 4-quinolyl group, a 5-quinolyl group, a 6-quinolyl group, a 7-quinolyl 20 group, an 8-quinolyl group, a 1-isoquinolyl group, a 3-isoquinolyl group, a 4-isoquinolyl group, a 5-isoquinolyl group, a 6-isoquinolyl group, a 7-isoquinolyl group, an 8-isoquinolyl group, a 2-quinoxalinyl group, a 5-quinoxalinyl group, a 6-quinoxalinyl group, a 1-carbazolyl group, a 2-car- 25 bazolyl group, a 3-carbazolyl group, a 4-carbazolyl group, a 9-carbazolyl group, a 1-phenanthridinyl group, a 2-phenanthridinyl group, a 3-phenanthridinyl group, a 4-phenanthridinyl group, a 6-phenanthridinyl group, a 7-phenanthridinyl group, an 8-phenanthridinyl group, a 9-phenanthridinyl 30 group, a 10-phenanthridinyl group, a 1-acridinyl group, a 2-acridinyl group, a 3-acridinyl group, a 4-acridinyl group, a 9-acridinyl group, a 1,7-phenanthrolin-2-yl group, a 1,7phenanthrolin-3-yl group, a 1,7-phenanthrolin-4-yl group, a 1,7-phenanthrolin-5-yl group, a 1,7-phenanthrolin-6-yl 35 group, a 1,7-phenanthrolin-8-yl group, a 1,7-phenanthrolin-9-yl group, a 1,7-phenanthrolin-10-yl group, a 1,8-phenanthrolin-2-yl group, a 1,8-phenanthrolin-3-yl group, a 1,8phenanthrolin-4-yl group, a 1,8-phenanthrolin-5-yl group, a 1,8-phenanthrolin-6-yl group, a 1,8-phenanthrolin-7-yl 40 group, a 1,8-phenanthrolin-9-yl group, a 1,8-phenanthrolin-10-yl group, a 1,9-phenanthrolin-2-yl group, a 1,9-phenanthrolin-3-yl group, a 1,9-phenanthrolin-4-yl group, a 1,9phenanthrolin-5-yl group, a 1,9-phenanthrolin-6-yl group, a 1,9-phenanthrolin-7-yl group, a 1,9-phenanthrolin-8-yl 45 group, a 1,9-phenanthrolin-10-yl group, a 1,10-phenanthrolin-2-yl group, a 1,10-phenanthrolin-3-yl group, a 1,10phenanthrolin-4-yl group, a 1,10-phenanthrolin-5-yl group, a 2,9-phenanthrolin-1-yl group, a 2,9-phenanthrolin-3-yl group, a 2,9-phenanthrolin-4-yl group, a 2,9-phenanthrolin-50 5-yl group, a 2,9-phenanthrolin-6-yl group, a 2,9-phenanthrolin-7-yl group, a 2,9-phenanthrolin-8-yl group, a 2,9phenanthrolin-10-yl group, a 2,8-phenanthrolin-1-yl group, a 2,8-phenanthrolin-3-yl group, a 2,8-phenanthrolin-4-yl group, a 2,8-phenanthrolin-5-yl group, a 2,8-phenanthrolin-55 6-yl group, a 2,8-phenanthrolin-7-yl group, a 2,8-phenanthrolin-9-yl group, a 2,8-phenanthrolin-10-yl group, a 2,7phenanthrolin-1-yl group, a 2,7-phenanthrolin-3-yl group, a 2,7-phenanthrolin-4-yl group, a 2,7-phenanthrolin-5-yl group, a 2,7-phenanthrolin-6-yl group, a 2,7-phenanthrolin-60 8-yl group, a 2,7-phenanthrolin-9-yl group, a 2,7-phenanthrolin-10-yl group, a 1-phenazinyl group, a 2-phenazinyl group, a 1-phenothiazinyl group, a 2-phenothiazinyl group, a 3-phenothiazinyl group, a 4-phenothiazinyl group, a 10-phenothiazinyl group, a 1-phenoxazinyl group, a 2-phenoxazinyl 65 group, a 3-phenoxazinyl group, a 4-phenoxazinyl group, a 10-phenoxazinyl group, a 2-oxazolyl group, a 4-oxazolyl

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group, a 5-oxazolyl group, a 2-oxadiazolyl group, a 5-oxadiazolyl group, a 3-furazanyl group, a 2-thienyl group, a 3-thienyl group, a 2-methylpyrrol-1-yl group, a 2-methylpyrrol-5-yl group, a 3-methylpyrrol-1-yl group, a 3-methylpyrrol-2-yl group, a 3-methylpyrrol-4-yl group, a 3-methylpyrrol-4-yl group, a 3-methylpyrrol-4-yl group, a 3-methylpyrrol-4-yl group, a 3-(2-phenylpropyl)pyrrol-1-yl group, a 2-methyl-1-indolyl group, a 4-methyl-1-indolyl group, a 2-methyl-3-indolyl group, a 4-t-butyl1-indolyl group, a 2-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 4-t-butyl3-indolyl group, and a 4-t-butyl3-indolyl group.

Examples of the substituted or unsubstituted alkyl group having 1 to 50 carbon atoms include a methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl group, an s-butyl group, an isobutyl group, a t-butyl group, an n-pentyl group, an n-hexyl group, an n-heptyl group, an n-octyl group, a hydroxymethyl group, a 1-hydroxyethyl group, a 2-hydroxyethyl group, a 2-hydroxyisobutyl group, a 1,2-dihydroxyethyl group, a 1,3-dihydroxyisopropyl group, a 2,3dihydroxy-t-butyl group, a 1,2,3-trihydroxypropyl group, a chloromethyl group, a 1-chloroethyl group, a 2-chloroethyl group, a 2-chloroisobutyl group, a 1,2-dichloroethyl group, a 1,3-dichloroisopropyl group, a 2,3-dichloro-t-butyl group, a 1,2,3-trichloropropyl group, a bromomethyl group, a 1-bromoethyl group, a 2-bromoethyl group, a 2-bromoisobutyl group, a 1,2-dibromoethyl group, a 1,3-dibromoisopropyl group, a 2,3-dibromo-t-butyl group, a 1,2,3-tribromopropyl group, an iodomethyl group, a 1-iodoethyl group, a 2-iodoethyl group, a 2-iodoisobutyl group, a 1,2-diiodoethyl group, a 1,3-diiodoisopropyl group, a 2,3-diiodo-t-butyl group, a 1,2,3-triiodopropyl group, an aminomethyl group, a 1-aminoethyl group, a 2-aminoethyl group, a 2-aminoisobutyl group, a 1,2-diaminoethyl group, a 1,3-diaminoisopropyl group, a 2,3-diamino-t-butyl group, a 1,2,3-triaminopropyl group, a cyanomethyl group, a 1-cyanoethyl group, a 2-cyanoethyl group, a 2-cyanoisobutyl group, a 1,2-dicyanoethyl group, a 1,3-dicyanoisopropyl group, a 2,3-dicyano-t-butyl group, a 1,2,3-tricyanopropyl group, a nitromethyl group, a 1-nitroethyl group, a 2-nitroethyl group, a 2-nitroisobutyl group, a 1,2-dinitroethyl group, a 1,3-dinitroisopropyl group, a 2,3-dinitro-t-butyl group, and 1,2,3-trinitropropyl group.

Examples of the substituted or unsubstituted cycloalkyl group having 3 to 50 carbon atoms include a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, a 4-methylcyclohexyl group, a 1-adamantyl group, a 2-adamantyl group, a 1-norbornyl group, and a 2-norbornyl group.

The substituted or unsubstituted alkoxy group having 1 to 50 carbon atoms is a group represented by —OY. Examples of Y include a methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl group, an s-butyl group, an isobutyl group, a t-butyl group, an n-pentyl group, an n-hexyl group, an n-heptyl group, an n-octyl group, a hydroxymethyl group, a 1-hydroxyethyl group, a 2-hydroxyethyl group, a 2-hydroxyisobutyl group, a 1,2-dihydroxyethyl group, a 1,3dihydroxyisopropyl group, a 2,3-dihydroxy-t-butyl group, a 1,2,3-trihydroxypropyl group, a chloromethyl group, a 1-chloroethyl group, a 2-chloroethyl group, a 2-chloroisobutyl group, a 1,2-dichloroethyl group, a 1,3-dichloroisopropyl group, a 2,3-dichloro-t-butyl group, a 1,2,3-trichloropropyl group, a bromomethyl group, a 1-bromoethyl group, a 2-bromoethyl group, a 2-bromoisobutyl group, a 1,2-dibromoethyl group, a 1,3-dibromoisopropyl group, a 2,3-dibromo-t-butyl group, a 1,2,3-tribromopropyl group, an iodomethyl group, a 1-iodoethyl group, a 2-iodoethyl group, a 2-iodoisobutyl group, a 1,2-diiodoethyl group, a 1,3-diiodoisopropyl group,

a 2,3-diiodo-t-butyl group, a 1,2,3-triiodopropyl group, an aminomethyl group, a 1-aminoethyl group, a 2-aminoethyl group, a 2-aminoisobutyl group, a 1,2-diaminoethyl group, a 1,3-diaminoisopropyl group, a 2,3-diamino-t-butyl group, a 1,2,3-triaminopropyl group, a cyanomethyl group, a 1-cyanoethyl group, a 2-cyanoethyl group, a 2-cyanoisobutyl group, a 1,2-dicyanoethyl group, a 1,3-dicyanoisopropyl group, a 2,3-dicyano-t-butyl group, a 1,2,3-tricyanopropyl group, a nitromethyl group, a 1-nitroethyl group, a 2-nitroet-1,3-dinitroisopropyl group, a 2,3-dinitro-t-butyl group, and 1,2,3-trinitropropyl group.

Examples of the substituted or unsubstituted aralkyl group having 7 to 50 carbon atoms include a benzyl group, a 1-phenylethyl group, a 2-phenylethyl group, a 1-phenylisopropyl group, a 2-phenylisopropyl group, a phenyl-t-butyl group, an α-naphthylmethyl group, a 1-α-naphthylethyl group, a 2-αnaphthylethyl group, a 1-α-naphthylisopropyl group, a 2-αnaphthylisopropyl group, a β-naphthylmethyl group, a 1-βnaphthylethyl group, a 2-β-naphthylethyl group, a 1-β- 20 naphthylisopropyl group, a 2-β-naphthylisopropyl group, a 1-pyrolylmethyl group, a 2-(1-pyrrolyl)ethyl group, a p-methylbenzyl group, an m-methylbenzyl group, an o-methylbenzyl group, a p-chlorobenzyl group, an m-chlorobenzyl group, an o-chlorobenzyl group, a p-bromobenzyl group, an 25 m-bromobenzyl group, an o-bromobenzyl group, a p-iodobenzyl group, an m-iodobenzyl group, an o-iodobenzyl group, a p-hydroxybenzyl group, an m-hydroxybenzyl group, an o-hydroxybenzyl group, a p-aminobenzyl group, an m-aminobenzyl group, an o-aminobenzyl group, a p-ni- 30 trobenzyl group, an m-nitrobenzyl group, an o-nitrobenzyl group, a p-cyanobenzyl group, an m-cyanobenzyl group, an o-cyanobenzyl group, a 1-hydroxy-2-phenylisopropyl group, and a 1-chloro-2-phenylisopropyl group.

Examples of the substituted or unsubstituted arvloxy group 35 having 6 to 50 carbon atoms forming the aromatic ring is represented by —OY'. Examples of Y' include a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, a 40 4-phenanthryl group, a 9-phenanthryl group, a 1-naphthacenyl group, a 2-naphthacenyl group, a 9-naphthacenyl group, a 1-pyrenyl group, a 2-pyrenyl group, a 4-pyrenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, a 45 p-terphenyl-2-yl group, an m-terphenyl-4-yl group, an m-terphenyl-3-yl group, an m-terphenyl-2-yl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl)phenyl group, a 3-methyl-2naphthyl group, a 4-methyl-1-naphthyl group, a 4-methyl-1- 50 anthryl group, a 4'-methylbiphenylyl group, and a 41'-t-butylp-terphenyl-4-yl group.

Examples of the substituted or unsubstituted heteroaryloxy group having 5 to 50 atoms forming the aromatic ring is represented by —OZ'. Examples of Z' include a 2-pyrrolyl 55 group, a 3-pyrrolyl group, a pyrazinyl group, a 2-pyridinyl group, a 3-pyridinyl group, a 4-pyridinyl group, a 2-indolyl group, a 3-indolyl group, a 4-indolyl group, a 5-indolyl group, a 6-indolyl group, a 7-indolyl group, a 1-isoindolyl group, a 3-isoindolyl group, a 4-isoindolyl group, a 5-isoin- 60 dolyl group, a 6-isoindolyl group, a 7-isoindolyl group, a 2-furyl group, a 3-furyl group, a 2-benzofuranyl group, a 3-benzofuranyl group, a 4-benzofuranyl group, a 5-benzofuranyl group, a 6-benzofuranyl group, a 7-benzofuranyl group, a 1-isobenzofuranyl group, a 3-isobenzofuranyl 65 group, a 4-isobenzofuranyl group, a 5-isobenzofuranyl group, a 6-isobenzofuranyl group, a 7-isobenzofuranyl

group, a 2-quinolyl group, a 3-quinolyl group, a 4-quinolyl group, a 5-quinolyl group, a 6-quinolyl group, a 7-quinolyl group, an 8-quinolyl group, a 1-isoquinolyl group, a 3-isoquinolyl group, a 4-isoquinolyl group, a 5-isoquinolyl group, a 6-isoquinolyl group, a 7-isoquinolyl group, an 8-isoquinolyl group, a 2-quinoxalinyl group, a 5-quinoxalinyl group, a 6-quinoxalinyl group, a 1-carbazolyl group, a 2-carbazolyl group, a 3-carbazolyl group, a 4-carbazolyl group, a 1-phenanthridinyl group, a 2-phenanthridinyl group, a hyl group, a 2-nitroisobutyl group, a 1,2-dinitroethyl group, a 10 3-phenanthridinyl group, a 4-phenanthridinyl group, a 6-phenanthridinyl group, a 7-phenanthridinyl group, an 8-phenanthridinyl group, a 9-phenanthridinyl group, a 10-phenanthridinyl group, a 1-acridinyl group, a 2-acridinyl group, a 3-acridinyl group, a 4-acridinyl group, a 9-acridinyl group, a 1,7-phenanthrolin-2-yl group, a 1,7-phenanthrolin-3-yl group, a 1,7-phenanthrolin-4-yl group, a 1,7-phenanthrolin-5-yl group, a 1,7-phenanthrolin-6-yl group, a 1,7phenanthrolin-8-yl group, a 1,7-phenanthrolin-9-yl group, a 1,7-phenanthrolin-10-yl group, a 1,8-phenanthrolin-2-yl group, a 1,8-phenanthrolin-3-yl group, a 1,8-phenanthrolin-4-yl group, a 1,8-phenanthrolin-5-yl group, a 1,8-phenanthrolin-6-yl group, a 1,8-phenanthrolin-7-yl group, a 1,8phenanthrolin-9-yl group, a 1,8-phenanthrolin-10-yl group, a 1,9-phenanthrolin-2-yl group, a 1,9-phenanthrolin-3-yl group, a 1,9-phenanthrolin-4-yl group, a 1,9-phenanthrolin-5-yl group, a 1,9-phenanthrolin-6-yl group, a 1,9-phenanthrolin-7-yl group, a 1,9-phenanthrolin-8-yl group, a 1,9phenanthrolin-10-yl group, a 1,10-phenanthrolin-2-yl group, a 1,10-phenanthrolin-3-yl group, a 1,10-phenanthrolin-4-yl group, a 1,10-phenanthrolin-5-yl group, a 2,9-phenanthrolin-1-yl group, a 2,9-phenanthrolin-3-yl group, a 2,9-phenanthrolin-4-yl group, a 2,9-phenanthrolin-5-yl group, a 2,9phenanthrolin-6-yl group, a 2,9-phenanthrolin-7-yl group, a 2,9-phenanthrolin-8-yl group, a 2,9-phenanthrolin-10-yl group, a 2,8-phenanthrolin-1-yl group, a 2,8-phenanthrolin-3-yl group, a 2,8-phenanthrolin-4-yl group, a 2,8-phenanthrolin-5-yl group, a 2,8-phenanthrolin-6-yl group, a 2,8phenanthrolin-7-yl group, a 2,8-phenanthrolin-9-yl group, a 2,8-phenanthrolin-10-yl group, a 2,7-phenanthrolin-1-yl group, a 2,7-phenanthrolin-3-yl group, a 2,7-phenanthrolin-4-yl group, a 2,7-phenanthrolin-5-yl group, a 2,7-phenanthrolin-6-yl group, a 2,7-phenanthrolin-8-yl group, a 2,7phenanthrolin-9-yl group, a 2,7-phenanthrolin-10-yl group, a 1-phenazinyl group, a 2-phenazinyl group, a 1-phenothiazinyl group, a 2-phenothiazinyl group, a 3-phenothiazinyl group, a 4-phenothiazinyl group, a 1-phenoxadinyl group, a 2-phenoxadinyl group, a 3-phenoxadinyl group, a 4-phenoxadinyl group, a 2-oxazolyl group, a 4-oxazolyl group, a 5-oxazolyl group, a 2-oxadiazolyl group, a 5-oxadiazolyl group, a 3-furazanyl group, a 2-thienyl group, a 3-thienyl group, a 2-methylpyrrol-1-yl group, a 2-methylpyrrol-3-yl group, a 2-methylpyrrol-4-yl group, a 2-methylpyrrol-5-yl group, a 3-methylpyrrol-1-yl group, a 3-methylpyrrol-2-yl group, a 3-methylpyrrol-4-yl group, a 3-methylpyrrol-5-yl group, a 2-t-butylpyrrol-4-yl group, a 3-(2-phenylpropyl)pyrrol-1-yl group, a 2-methyl-1-indolyl group, a 4-methyl-1indolyl group, a 2-methyl-3-indolyl group, a 4-methyl-3-indolyl group, a 2-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 2-t-butyl3-indolyl group, and a 4-t-butyl3-indolyl group.

> The substituted or unsubstituted arylthio group having 6 to 50 carbon atoms forming the aromatic ring is represented by -SY". Examples of Y" include a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, a 4-phenanthryl group, a 9-phenanthryl group, a 1-naphthacenyl group, a 2-naphthace-

nyl group, a 9-naphthacenyl group, a 1-pyrenyl group, a 2-pyrenyl group, a 4-pyrenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, a p-terphenyl-2-yl group, an m-terphenyl-3-yl group, an m-terphenyl-2-yl group, an m-terphenyl-2-yl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl) phenyl group, a 3-methyl-2-naphthyl group, a 4-methyl-1-naphthyl group, a 4-methyl-1-anthryl group, a 4'-methylbiphenylyl group, and a 4"-t-butyl-p-terphenyl-4-yl group.

The substituted or unsubstituted heteroarylthio group having 5 to 50 atoms forming the aromatic ring is represented by -SZ". Examples of Z" include a 2-pyrrolyl group, a 3-pyrrolyl group, a pyrazinyl group, a 2-pyridinyl group, a 3-pyridinyl group, a 4-pyridinyl group, a 2-indolyl group, a 3-indolyl group, a 4-indolyl group, a 5-indolyl group, a 6-indolyl group, a 7-indolyl group, a 1-isoindolyl group, a 3-isoindolyl group, a 4-isoindolyl group, a 5-isoindolyl group, a 6-isoindolyl group, a 7-isoindolyl group, a 2-furyl group, a 3-furyl group, a 2-benzofuranyl group, a 3-benzofuranyl group, a 20 4-benzofuranyl group, a 5-benzofuranyl group, a 6-benzofuranyl group, a 7-benzofuranyl group, a 1-isobenzofuranyl group, a 3-isobenzofuranyl group, a 4-isobenzofuranyl group, a 5-isobenzofuranyl group, a 6-isobenzofuranyl group, a 7-isobenzofuranyl group, a 2-quinolyl group, a 25 3-quinolyl group, a 4-quinolyl group, a 5-quinolyl group, a 6-quinolyl group, a 7-quinolyl group, an 8-quinolyl group, a 1-isoquinolyl group, a 3-isoquinolyl group, a 4-isoquinolyl group, a 5-isoquinolyl group, a 6-isoquinolyl group, a 7-isoquinolyl group, an 8-isoquinolyl group, a 2-quinoxalinyl 30 group, a 5-quinoxalinyl group, a 6-quinoxalinyl group, a 1-carbazolyl group, a 2-carbazolyl group, a 3-carbazolyl group, a 4-carbazolyl group, a 1-phenanthridinyl group, a 2-phenanthridinyl group, a 3-phenanthridinyl group, a 4-phenanthridinyl group, a 6-phenanthridinyl group, a 35 7-phenanthridinyl group, an 8-phenanthridinyl group, a 9-phenanthridinyl group, a 10-phenanthridinyl group, a 1-acridinyl group, a 2-acridinyl group, a 3-acridinyl group, a 4-acridinyl group, a 9-acridinyl group, a 1,7-phenanthrolin-2-yl group, a 1,7-phenanthrolin-3-yl group, a 1,7-phenan- 40 throlin-4-yl group, a 1,7-phenanthrolin-5-yl group, a 1,7phenanthrolin-6-yl group, a 1,7-phenanthrolin-8-yl group, a 1,7-phenanthrolin-9-yl group, a 1,7-phenanthrolin-10-yl group, a 1,8-phenanthrolin-2-yl group, a 1,8-phenanthrolin-3-yl group, a 1,8-phenanthrolin-4-yl group, a 1,8-phenan- 45 throlin-5-yl group, a 1,8-phenanthrolin-6-yl group, a 1,8phenanthrolin-7-yl group, a 1,8-phenanthrolin-9-yl group, a 1,8-phenanthrolin-10-yl group, a 1,9-phenanthrolin-2-yl group, a 1,9-phenanthrolin-3-yl group, a 1,9-phenanthrolin-4-yl group, a 1,9-phenanthrolin-5-yl group, a 1,9-phenan- 50 throlin-6-yl group, a 1,9-phenanthrolin-7-yl group, a 1,9phenanthrolin-8-yl group, a 1,9-phenanthrolin-10-yl group, a 1,10-phenanthrolin-2-yl group, a 1,10-phenanthrolin-3-yl group, a 1,10-phenanthrolin-4-yl group, a 1,10-phenanthrolin-5-yl group, a 2,9-phenanthrolin-1-yl group, a 2,9-phenan- 55 throlin-3-yl group, a 2,9-phenanthrolin-4-yl group, a 2,9phenanthrolin-5-yl group, a 2,9-phenanthrolin-6-yl group, a 2,9-phenanthrolin-7-yl group, a 2,9-phenanthrolin-8-yl group, a 2,9-phenanthrolin-10-yl group, a 2,8-phenanthrolin-1-yl group, a 2,8-phenanthrolin-3-yl group, a 2,8-phenan- 60 throlin-4-yl group, a 2,8-phenanthrolin-5-yl group, a 2,8phenanthrolin-6-yl group, a 2,8-phenanthrolin-7-yl group, a 2,8-phenanthrolin-9-yl group, a 2,8-phenanthrolin-10-yl group, a 2,7-phenanthrolin-1-yl group, a 2,7-phenanthrolin-3-yl group, a 2,7-phenanthrolin-4-yl group, a 2,7-phenan- 65 throlin-5-yl group, a 2,7-phenanthrolin-6-yl group, a 2,7phenanthrolin-8-yl group, a 2,7-phenanthrolin-9-yl group, a

2,7-phenanthrolin-10-yl group, a 1-phenazinyl group, a 2-phenazinyl group, a 1-phenothiazinyl group, a 2-phenothiazinyl group, a 3-phenothiazinyl group, a 4-phenothiazinyl group, a 1-phenoxazinyl group, a 2-phenoxazinyl group, a 3-phenoxazinyl group, a 4-phenoxazinyl group, a 2-oxazolyl group, a 4-oxazolyl group, a 5-oxazolyl group, a 2-oxadiazolyl group, a 5-oxadiazolyl group, a 3-furazanyl group, a 2-thienyl group, a 3-thienyl group, a 2-methylpyrrol-1-yl group, a 2-methylpyrrol-3-yl group, a 2-methylpyrrol-4-yl group, a 2-methylpyrrol-5-yl group, a 3-methylpyrrol-1-yl group, a 3-methylpyrrol-2-yl group, a 3-methylpyrrol-4-yl group, a 3-methylpyrrol-5-yl group, a 2-t-butylpyrrol-4-yl group, a 3-(2-phenylpropyl)pyrrol-1-yl group, a 2-methyl-1indolyl group, a 4-methyl-1-indolyl group, a 2-methyl-3-indolyl group, a 4-methyl-3-indolyl group, a 2-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 2-t-butyl3-indolyl group, and a 4-t-butyl3-indolyl group.

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The substituted or unsubstituted alkoxycarbonyl group having 2 to 50 carbon atoms is represented by —COOZ. Examples of Z include a methyl group, an ethyl group, a propyl group, an isopropyl group, an n-butyl group, an s-butyl group, an isobutyl group, a t-butyl group, an n-pentyl group, an n-hexyl group, an n-heptyl group, an n-octyl group, a hydroxymethyl group, a 1-hydroxyethyl group, a 2-hydroxyethyl group, a 2-hydroxyisobutyl group, a 1,2-dihydroxyethyl group, a 1,3-dihydroxyisopropyl group, a 2,3-dihydroxy-tbutyl group, a 1,2,3-trihydroxypropyl group, a chloromethyl group, a 1-chloroethyl group, a 2-chloroethyl group, a 2-chloroisobutyl group, a 1,2-dichloroethyl group, a 1,3dichloroisopropyl group, a 2,3-dichloro-t-butyl group, a 1,2, 3-trichloropropyl group, a bromomethyl group, a 1-bromoethyl group, a 2-bromoethyl group, a 2-bromoisobutyl group, a 1,2-dibromoethyl group, a 1,3-dibromoisopropyl group, a 2,3-dibromo-t-butyl group, a 1,2,3-tribromopropyl group, an iodomethyl group, a 1-iodoethyl group, a 2-iodoethyl group, a 2-iodoisobutyl group, a 1,2-diiodoethyl group, a 1,3-diiodoisopropyl group, a 2,3-diiodo-t-butyl group, a 1,2,3-triiodopropyl group, an aminomethyl group, a 1-aminoethyl group, a 2-aminoethyl group, a 2-aminoisobutyl group, a 1,2-diaminoethyl group, a 1,3-diaminoisopropyl group, a 2,3-diamino-t-butyl group, a 1,2,3-triaminopropyl group, a cyanomethyl group, a 1-cyanoethyl group, a 2-cyanoethyl group, a 2-cyanoisobutyl group, a 1,2-dicyanoethyl group, a 1,3-dicyanoisopropyl group, a 2,3-dicyano-t-butyl group, a 1,2,3-tricyanopropyl group, a nitromethyl group, a 1-nitroethyl group, a 2-nitroethyl group, a 2-nitroisobutyl group, a 1,2-dinitroethyl group, a 1,3-dinitroisopropyl group, a 2,3dinitro-t-butyl group, and 1,2,3-trinitropropyl group.

The substituted or unsubstituted aryl group having 6 to 50 carbon atoms forming the aromatic ring or an amino group substituted with a substituted or unsubstituted heteroaryl group having 5 to 50 atoms forming the aromatic ring is represented by —NPQ. Examples of P and Q include a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, 4-phenanthryl group, a 9-phenanthryl group, a 1-naphthacenyl group, a 2-naphthacenyl group, a 9-naphthacenyl group, a 1-pyrenyl group, a 2-pyrenyl group, a 4-pyrenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, a p-terphenyl-2-yl group, an m-terphenyl-4-yl group, a an m-terphenyl-3-yl group, an m-terphenyl-2-yl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl)phenyl group, a 3-methyl-2-naphthyl group, a 4-methyl-1-naphthyl group, a 4-methyl-1-anthryl group, a 4'-methylbiphenylyl group, and a 4"-tbutyl-p-terphenyl-4-yl group, a 2-pyrrolyl group, a 3-pyrrolyl group, a pyrazinyl group, a 2-pyridinyl group, a 3-pyridinyl group, a 4-pyridinyl group, a 2-indolyl group, a 3-indolyl group, a 4-indolyl group, a 5-indolyl group, a 6-indolyl group, a 7-indolyl group, a 1-isoindolyl group, a 3-isoindolyl 5 group, a 4-isoindolyl group, a 5-isoindolyl group, a 6-isoindolyl group, a 7-isoindolyl group, a 2-furyl group, a 3-furyl group, a 2-benzofuranyl group, a 3-benzofuranyl group, a 4-benzofuranyl group, a 5-benzofuranyl group, a 6-benzofuranyl group, a 7-benzofuranyl group, a 1-isobenzofuranyl 10 group, a 3-isobenzofuranyl group, a 4-isobenzofuranyl group, a 5-isobenzofuranyl group, a 6-isobenzofuranyl group, a 7-isobenzofuranyl group, a 2-quinolyl group, a 3-quinolyl group, a 4-quinolyl group, a 5-quinolyl group, a 6-quinolyl group, a 7-quinolyl group, an 8-quinolyl group, a 15 1-isoquinolyl group, a 3-isoquinolyl group, a 4-isoquinolyl group, a 5-isoquinolyl group, a 6-isoquinolyl group, a 7-isoquinolyl group, an 8-isoquinolyl group, a 2-quinoxalinyl group, a 5-quinoxalinyl group, a 6-quinoxalinyl group, a 1-carbazolyl group, a 2-carbazolyl group, a 3-carbazolyl 20 group, a 4-carbazolyl group, a 1-phenanthridinyl group, a 2-phenanthridinyl group, a 3-phenanthridinyl group, a 4-phenanthridinyl group, a 6-phenanthridinyl group, a 7-phenanthridinyl group, an 8-phenanthridinyl group, a 9-phenanthridinyl group, a 10-phenanthridinyl group, a 25 1-acridinyl group, a 2-acridinyl group, a 3-acridinyl group, 4-acridinyl group, a 9-acridinyl group, a 1,7-phenanthrolin-2-yl group, a 1,7-phenanthrolin-3-yl group, a 1,7-phenanthrolin-4-yl group, a 1,7-phenanthrolin-5-yl group, a 1,7phenanthrolin-6-yl group, a 1,7-phenanthrolin-8-yl group, a 30 1,7-phenanthrolin-9-yl group, a 1,7-phenanthrolin-10-yl group, a 1,8-phenanthrolin-2-yl group, a 1,8-phenanthrolin-3-yl group, a 1,8-phenanthrolin-4-yl group, a 1,8-phenanthrolin-5-yl group, a 1,8-phenanthrolin-6-yl group, a 1,8phenanthrolin-7-yl group, a 1,8-phenanthrolin-9-yl group, a 35 1,8-phenanthrolin-10-yl group, a 1,9-phenanthrolin-2-yl group, a 1,9-phenanthrolin-3-yl group, a 1,9-phenanthrolin-4-yl group, a 1,9-phenanthrolin-5-yl group, a 1,9-phenanthrolin-6-yl group, a 1,9-phenanthrolin-7-yl group, a 1,9phenanthrolin-8-yl group, a 1,9-phenanthrolin-10-yl group, a 40 1,10-phenanthrolin-2-yl group, a 1,10-phenanthrolin-3-yl group, a 1,10-phenanthrolin-4-yl group, a 1,10-phenanthrolin-5-yl group, a 2,9-phenanthrolin-1-yl group, a 2,9-phenanthrolin-3-yl group, a 2,9-phenanthrolin-4-yl group, a 2,9phenanthrolin-5-yl group, a 2,9-phenanthrolin-6-yl group, a 45 2,9-phenanthrolin-7-yl group, a 2,9-phenanthrolin-8-yl group, a 2,9-phenanthrolin-10-yl group, a 2,8-phenanthrolin-1-yl group, a 2,8-phenanthrolin-3-yl group, a 2,8-phenanthrolin-4-yl group, a 2,8-phenanthrolin-5-yl group, a 2,8phenanthrolin-6-yl group, a 2,8-phenanthrolin-7-yl group, a 50 2,8-phenanthrolin-9-yl group, a 2,8-phenanthrolin-10-yl group, a 2,7-phenanthrolin-1-yl group, a 2,7-phenanthrolin-3-yl group, a 2,7-phenanthrolin-4-yl group, a 2,7-phenanthrolin-5-yl group, a 2,7-phenanthrolin-6-yl group, a 2,7phenanthrolin-8-yl group, a 2,7-phenanthrolin-9-yl group, a 55 2,7-phenanthrolin-10-yl group, a 1-phenazinyl group, a 2-phenazinyl group, a 1-phenothiazinyl group, a 2-phenothiazinyl group, a 3-phenothiazinyl group, a 4-phenothiazinyl group, a 1-phenoxazinyl group, a 2-phenoxazinyl group, a 3-phenoxazinyl group, a 4-phenoxazinyl group, a 2-oxazolyl 60 group, a 4-oxazolyl group, a 5-oxazolyl group, a 2-oxadiazolyl group, a 5-oxadiazolyl group, a 3-furazanyl group, a 2-thienyl group, a 3-thienyl group, a 2-methylpyrrol-1-yl group, a 2-methylpyrrol-3-yl group, a 2-methylpyrrol-4-yl group, a 2-methylpyrrol-5-yl group, a 3-methylpyrrol-1-yl 65 group, a 3-methylpyrrol-2-yl group, a 3-methylpyrrol-4-yl

group, a 3-methylpyrrol-5-yl group, a 2-t-butylpyrrol-4-yl

group, a 3-(2-phenylpropyl)pyrrol-1-yl group, a 2-methyl-1-indolyl group, a 4-methyl-1-indolyl group, a 2-methyl-3-indolyl group, a 4-methyl-3-indolyl group, a 2-t-butyl1-indolyl group, a 4-t-butyl1-indolyl group, a 4-t-butyl3-indolyl group, and a 4-t-butyl3-indolyl group.

Specific examples of the compound represented by the general formula (I) are shown below. However, the present invention is not limited to these examples.

[Chem 147]

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-continued

In addition, an aromatic amine represented by the following general formula (II) is also suitably used in the formation of the hole injecting layer or hole transporting layer.

[Chem 148]

$$\begin{array}{c} Ar_1 \\ A_2 - N \\ Ar_3 \end{array} \tag{II)}$$

In the general formula (II), the definition of Ar_1 to Ar_3 is the same as that of Ar^1 to Ar^4 in the general formula (I). Specific examples of the compound represented by the general formula (II) are shown below. However, the present invention is not limited to these examples.

[Chem 149]

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The compound of the present invention can be used in each of the hole injecting layer, the hole transporting layer, the electron injecting layer, and the electron transporting layer because the compound can transport both a hole and an electron.

In the present invention, the anode in the organic EL device has the function of injecting holes into the hole transporting layer or the light emitting layer. It is effective that the anode has a work function of 4.5 eV or greater. Specific examples of the material for the anode used in the present invention include indium tin oxide alloys (ITO), tin oxide (NESA), gold, silver, platinum, and copper. In addition, as the cathode, a material having a small work function is preferred in view to inject an electron into an electron injecting layer or a light emitting layer. Examples of the cathode material are not particularly limited, and specifically, indium, aluminum, magnesium, an magnesium-indium alloy, a magnesium-aluminum alloy, an aluminum-lithium alloy, an aluminum-scandium-lithium alloy, and a magnesium-silver alloy may be used.

The method of forming the layers in the organic EL device of the present invention is not particularly limited. A conventionally known process such as the vacuum vapor deposition for process or the spin coating process can be used. The organic thin film layer which is used in the organic EL device of the present invention and includes the compound represented by general formula (1) described above can be formed in accordance with a known process such as the vacuum vapor deposition process or the molecular beam epitaxy process (MBE process) or, using a solution prepared by dissolving the com-

pounds into a solvent, in accordance with a coating process such as the dipping process, the spin coating process, the casting process, the bar coating process, or the roll coating process.

The thickness of each organic layer in the organic EL device of the present invention is not particularly limited. In general, an excessively thin layer tends to have defects such as pin holes, whereas an excessively thick layer requires a high applied voltage to decrease the efficiency. Therefore, a thickness in the range of several nanometers to 1 µm is preferable.

EXAMPLES

Next, the present invention is described in detail by way of examples, but the present invention is not limited to the following examples. Note that, in the synthesis examples below, DMF refers to dimethylformamide, THF refers to tetrahydrofuran, DME refers to dimethoxyethane, NBS refers to N-bromosuccine imide, Ph refers to a phenyl group, AcOEt refers to ethyl acetate, and NMP refers to N-methylpyrrolidone.

Synthesis Example 1-1

Synthesis of Compound 1-1

(1) Synthesis of Compound A-1

1,4-dibromo-2,5-difluorobenzene (49.3 g, 181.5 mmol), 2-methoxyphenylboronic acid (66.2 g, 435.6 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (363 mL, 726 mmol), DME (360 mL), toluene (360 mL), and $\rm Pd[PPh_3]_4$ (21 g, 18.0 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (500 mL) was charged into the funnel. Then, the mixture was extracted with CH $_2$ Cl $_2$. The extract was dried with MgSO $_4$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 38.5 g in 65% yield.

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(2) Synthesis of Compound A-2

Compound A-1 (36.6 g, 112.1 mmol), NBS (39.9 g, 224 35 mmol), and DMF (1,000 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at room temperature for 8 hours. After the completion of the reaction, the resultant sample was transferred to a separating funnel, and water (1,000 mL) was charged into the funnel. Then, the mixture was extracted with AcOEt. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 38 g in 70% yield.

FD-MS $\rm C_{20}H_{14}Br_2F_2O_2$: theoretical value 484, observed $\rm \ _{45}$ value 484

(3) Synthesis of Compound A-3

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Compound A-2 (37.2 g, 76.7 mmol), a 1-M solution of BBr₃ in CH₂Cl₂ (180 mL, 180 mmol), and CH₂Cl₂ (500 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO₃. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 28 g in 80% yield.

FD-MS $\rm C_{18}H_{10}Br_2F_2O_2$: theoretical value 456, observed value 456

Synthesis of Compound A-4

[Chem 153]

Br

OH

$$K_2CO_3$$
 NMP

Br

Compound A-3 (27.4 g, 60 mmol), K₂CO₃ (18.2 g, 132 mmol), and NMP (250 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 150° C. for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (500

mL) was charged into the funnel. Then, the mixture was extracted with AcOEt. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 20 g in 80% yield.

FD-MS $C_{18}H_8Br_2O_2$: theoretical value 416, observed ⁵ value 416

(5) Synthesis of Compound 1-1

Compound A-4 (3 g, 7.2 mmol), carbazole (2.9 g, 17.3 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), K₃PO₄ (6.1 g, 28.8 mmol), and 1,4dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged 60 into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-1) was obtained. The powder was puri- 65 fied by sublimation, whereby a white solid was obtained in an amount of 2.2 g in 52% yield.

FD-MS $C_{42}H_{24}N_2O_2$: theoretical value 588, observed value 588

Synthesis Example 1-2

Synthesis of Compound 1-17

(1) Synthesis of Compound A-5

Compound A-4 (3 g, 7.2 mmol), carbazole (1.5 g, 7.2 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), K₃PO₄ (6.1 g, 28.8 mmol), and 1,4dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 2.2 g in 60% yield.

FD-MS C₃₀H₁₆BrNO₂: theoretical value 502, observed value 502

(2) Synthesis of Compound 1-17

trated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-17) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.0 g in 45% yield. FD-MS $C_{54}H_{32}N_2O_2$: theoretical value 740, observed value 740

[Chem 156] 10 $(HO)_2B$ $Pd[PPh_{3}]_{4} \\$ Na₂CO₃ 2M aq. DME/Toluene

Compound A-5 (3.0 g, 6.0 mmol), Compound A-6 (2.4 g, 6.6 mmol), a 2 M aqueous solution of Na₂CO₃ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh₃]₄ (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

1-17

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and 65 concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concen-

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Synthesis Example 1-3

Synthesis of Compound 1-18

Compound A-5 (3.3 g, 6.6 mmol), Compound A-7 (2.1 g, 7.3 mmol), a 2 M aqueous solution of Na₂CO₃ (6 mL, 13 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh₃]₄ (0.38 g, 0.33 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel

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added thereto, followed by extraction with CH2Cl2. An

organic layer was washed with a saturated NaNO2 aqueous

column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-18) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.3 g in 52% yield.

FD-MS C₄₈H₂₇NO₃: theoretical value 665, observed value 665

Synthesis Example 1-4

Synthesis of Compound 1-34

(1) Synthesis of Compound A-8

solution (50 mL) and dried with MgSO₄, followed by filtration and concentration. The sample was purified by a column chromatography, whereby a white solid was obtained in an amount of 7.9 g in 62% yield. FD-MS $C_{42}H_{22}Br_2N_2O_2$: theoretical value 746, observed 10 value 746

(2) Synthesis of Compound 1-34

[Chem 159] [Chem 158]

$$\frac{Br_2}{CH_2Cl_2}$$

Compound (1-1) (10 g, 17 mmol) and CH₂Cl₂ (100 mL) were loaded into a three-necked flask and bromine (5.4 g, 34 mmol) was dropped thereto under an Ar atmosphere at $0^{\rm o}$ C. $_{65}$ After that, the mixture was stirred at room temperature for 8 hours. After the completion of the reaction, the sample was

 $(HO)_2B$

1-34

Pd[PPh₃]₄ Na₂CO₃ 2M aq. Compound A-8 (3.7 g, 4.9 mmol), phenylboronic acid (1.32 g, 10.8 mmol), a 2 M aqueous solution of $\mathrm{Na_2CO_3}$ (5 mL, 9.8 mmol), DME (10 mL), toluene (10 mL), and Pd[PPh_3]_4 (0.29 g, 0.25 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. 10 The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-34) was obtained. The powder 15 was purified by sublimation, whereby a white solid was obtained in an amount of 1.8 g in 50% yield.

FD-MS $C_{54}H_{32}N_2O_2$: theoretical value 740, observed value 740

Synthesis Example 1-5

Synthesis of Compound 1-46

(1) Synthesis of Compound A-9

[Chem 160]

-continued

Compound A-5 (10 g, 20 mmol) and THF (200 mL) were loaded into a three-necked flask, and the mixture was cooled to -78° C. Then, n-BuLi (1.65-M solution in n-hexane, 13.3 mL, 22 mmol) was added dropwise to the flask, and the ²⁵ resultant mixture was stirred at -78° C. for 20 minutes. Triisopropyl boronate (11.3 g, 60 mmol) was added to the resultant, and the mixture was stirred at -78° C. for 1 hour. After that, the resultant was left to stand overnight at room temperature. Then, 1N HCl (40 mL) was charged into the resultant, and the mixture was stirred at room temperature for 1 hour. The resultant sample was concentrated, and was then transferred to a separating funnel. Water (50 mL) was charged into the funnel, and the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by recrystallization (toluene-hexane), whereby a white solid was obtained in an amount of 5.6 g in 600 yield.

(2) Synthesis of Compound 1-46

-continued

Compound A-5 (3.1 g, 6.2 mmol), Compound A-9 (3.2 g, 6.8 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6.2 mL, 12.4 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh_3]_4 (0.36 g, 0.31 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel

column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-46) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.1 g in 40% yield.

FD-MS $C_{60}H_{32}N_2O_4$: theoretical value 844, observed value 844

Synthesis Example 1-6

Synthesis of Compound 1-49

A-9

1-49

Compound A-9 (10.2 g, 21.9 mmol), 1,3,5-tribromobenzene (2.3 g, 7.3 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (22.5 mL, 45 mmol), DME (15 mL), toluene (15 mL), and 35 Pd[PPh₃]₄ (0.63 g, 0.56 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with $\mathrm{MgSO_4}$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-49) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.6 g in 16% yield.

FD-MS $C_{96}H_{51}N_3O_6$: theoretical value 1,342 observed 50 value 1,342

Synthesis Example 1-7

Synthesis of Compound 1-68

Compound A-10 (3 g, 7.2 mmol), carbazole (3.0 g, 14.4 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), $\rm K_3PO_4$ (6.1 g, 28.8 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂.

The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-68) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.2 g in 52% yield.

FD-MS $C_{42}H_{24}\bar{N_2}O_2;$ theoretical value 588, observed value 588

Synthesis Example 1-8

Synthesis of Compound 1-74

[Chem 164]

Compound A-11 (3.7 g, 4.9 mmol), Compound A-6 (2.0 g, $_{\rm 40}$ 5.4 mmol), a 2 M aqueous solution of Na₂CO₃ (5 mL, 9.8 mmol), DME (10 mL), toluene (10 mL), and Pd[PPh₃]₄ (0.29 g, 0.25 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel

A-11

[Chem 165]

column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-74) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.8 g in 50% yield.

1-74

478

FD-MS $C_{54}H_{32}N_2O_2$: theoretical value 740, observed value 740

Synthesis Example 1-9

Synthesis of Compound 1-85

Compound A-11 (3.0 g, 6.0 mmol), Compound A-7 (1.9 g, 6.6 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh₃]₄ (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-85) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.2 g in 55% yield.

FD-MS $\rm C_{48}H_{27}NO_3$: theoretical value 665, observed value 665

Synthesis Example 1-10

Synthesis of Compound 1-87

Compound A-12 (3.3 g, 5.0 mmol), phenylboronic acid (0.67 g, 5.5 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (5 mL, 10 mmol), DME (10 mL), toluene (10 mL), and Pd[PPh_3]_4 (0.29 g, 0.25 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-87) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.5 g in 45% yield.

FD-MS $C_{48}H_{28}N_2O_2$: theoretical value 664, observed value 664

Synthesis Example 1-11

Synthesis of Compound 1-113

Compound A-11 (109 g, 20 mmol) and THF (200 mL) were loaded into a three-necked flask, and the mixture was cooled to -78° C. Then, n-BuLi (1.65-M solution in n-hexane, 13.3 mL, 22 mmol) was added dropwise to the flask, and the resultant mixture was stirred at -78° C. for 20 minutes. Triisopropyl boronate (11.3 g, 60 mmol) was added to the resultant, and the mixture was stirred at -78° C. for 1 hour. After that, the resultant was left to stand overnight at room temperature. Then, 1N HCl (40 mL) was charged into the 10 resultant, and the mixture was stirred at room temperature for 1 hour. The resultant sample was concentrated, and was then transferred to a separating funnel. Water (50 mL) was charged into the funnel, and the mixture was extracted with CH2Cl2. The extract was dried with $MgSO_4$, and was then filtrated and 15 concentrated. The resultant sample was purified by recrystallization (toluene-hexane), whereby a white solid was obtained in an amount of 5.0 g in 540 yield.

2) Synthesis of Compound 1-113

Compound A-11 (3.0 g, 6.0 mmol), Compound A-13 (3.1 g, 6.6 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6.0 mL, 12 mmol), DME (12 mL), toluene (12 mL), and $\rm Pd[PPh_3]_4$ (0.35 g, 0.30 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-113) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.8 g in 56% yield.

FD-MS $\rm C_{60}H_{32}N_2O_4$: theoretical value 844, observed value 844

$$B(OH)_2$$

A-13

1-113

Synthesis of Compound 1-116

Compound A-13 (10.2 g, 21.9 mmol), 1,3,5-tribromobenzene (2.3 g, 7.3 mmol), a 2 M aqueous solution of Na₂CO₃ (22.5 mL, 45 mmol), DME (15 mL), toluene (15 mL), and Pd[PPh₃]₄ (0.63 g, 0.56 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged 55 into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-116) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.3 g in 13% yield.

FD-MS $\rm C_{96}H_{51}N_3O_6:$ theoretical value 1,342, observed value 1,342

Synthesis Example 1-13

Synthesis of Compound 1-138

(1) Synthesis of Compound A-15

[Chem 170]

$$B(OH)_2$$
14

-continued
$$\begin{array}{c} F \\ F \\ Na_2CO_3 \ 2M \ aq. \\ \hline DME/Toluene \\ \\ S \\ \hline \\ O_2N \\ \hline \\ Br \\ \\ 15 \\ \end{array}$$

Compound A-14 (24.6 g, 74 mmol), 1,4-dibromo-2,5-difluorobenzene (20 g, 74 mmol), and a 2 M aqueous solution of $\rm Na_2CO_3$ (75 mL, 150 mmol), DME (150 mL), toluene (150 mL), and Pd[PPh $_3$] $_4$ (4.3 g, 3.7 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar 25 atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with $\rm CH_2Cl_2$. The extract was dried with $\rm MgSO_4$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 21 g in 60% yield.

FD-MS $\rm C_{24}H_{13}BrF_2N_2O_2$: theoretical value 479, observed $\,$ 35 value 479

(2) Synthesis of Compound A-17

[Chem 171]

A-16

Compound A-15 (20.1 g, 42 mmol), Compound A-16 (14.6 g, 46 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (42 mL, 84 mmol), DME (85 mL), toluene (85 mL), and $\rm Pd[PPh_3]_4$ (2.4 g, 2.1 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 15.5 g in 55% yield.

FD-MS $\rm C_{43}H_{27}F_2N_3O_3:$ theoretical value 671, observed value 671

(3) Synthesis of Compound A-18

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Compound A-17 (15.0 g, 22.3 mmol), a 1-M solution of in CH₂Cl₂ (100 mL, 100 mmol), and CH₂Cl₂ (200 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO₃. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained 35 in an amount of 12.5 g in 85% yield.

FD-MS $\rm C_{42}H_{25}F_2N_3O_3$: theoretical value 657, observed value 657

(4) Synthesis of Compound A-19

Compound A-18 (12.0 g, 18.2 mmol), 5% Ru—C (0.73 g), and ethanol (68 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 70° C. Hydrazine monohydrate (5.5 g, 110 mmol) was dissolved in ethanol (6 mL) and dropped thereto. After that, the reaction mixture was refluxed for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The sample was filtrated under reduced pressure, and the filtrate was concentrated. The sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 9.7 g in 85% yield.

FD-MS $\rm C_{42}H_{27}F_2N_3O$: theoretical value 627, observed value 627

(5) Synthesis of Compound A-20

Compound A-19 (9.7 g, 15.5 mmol), K₂CO₃ (4.7 g, 34.1 mmol), and NMP (50 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 25 $150^{\rm o}$ C. for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by 30 column chromatography, whereby a white solid was obtained in an amount of 7.3 g in 80% yield.

FD-MS C₄₂H₂₅N₃O: theoretical value 587, observed value 587

(6) Synthesis of Compound 1-138

Compound A-20 (5.0 g, 8.5 mmol), iodobenzene (1.7 g, 8.5 mmol), CuI (1.6 g, 8.5 mmol), transcyclohexane 1,2-diamine (2.9 g, 25.5 mmol), K₃PO₄ (7.2 g, 34 mmol), and 1,4-dioxane (9 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-138) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.8 g in 50% yield.

FD-MS $C_{48}H_{29}N_{30}$: theoretical value 663, observed value

[Chem 175]

Synthesis Example 1-14

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[Chem 176]

Synthesis of Compound 1-140

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Compound A-21 (2.8 g, 7.3 mmol), carbazole (2.4 g, 14.6 mmol), CuI (1.4 g, 7.3 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.9 mmol), K_3PO_4 (6.2 g, 29.2 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the 25 mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\rm CH_2Cl_2$. 30 The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-140) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.3 g in 52% yield.

FD-MS $\rm C_{42}H_{24}N_2OS:$ theoretical value 604, observed value 604

Synthesis Example 1-15

Synthesis of Compound 1-148

(1) Synthesis of Compound A-23

[Chem 177]

-continued

Br

CuI,

NH2

K₃PO₄

Dioxane, reflux

A-23

Compound A-22 (5.0 g, 8.5 mmol), 2-bromobenzofuran (2.1 g, 8.5 mmol), CuI (1.6 g, 8.5 mmol), transcyclohexane 1,2-diamine (2.9 g, 25.5 mmol), ${\rm K_3PO_4}$ (7.2 g, 34 mmol), and 1,4-dioxane (9 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 2.4 g in 37% yield.

FD-MS $\rm C_{54}H_{32}N_{40}$: theoretical value 752, observed value 752

(2) Synthesis of Compound 1-148

[Chem 178]
50
60
A-23

Compound A-23 (2.4 g, 3.2 mmol), iodobenzene (0.65 g, 3.2 mmol), CuI (0.61 g, 3.2 mmol), transcyclohexane 1,2diamine (1.1 g, 9.6 mmol), K₃PO₄ (2.7 g, 12.8 mmol), and 1,4-dioxane (4 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10

After the completion of the reaction, the resultant was 35 cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-148) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.4 g in 53% yield.

FD-MS $C_{60}H_{36}N_{40}$: theoretical value 828, observed value $_{45}$

Synthesis Example 1-16

Synthesis of Compound 1-149

Compound A-24 (4.2 g, 10 mmol), 2-bromobenzofuran (5.0 g, 20 mmol), CuI (1.9 g, 10 mmol), transcyclohexane 1,2-diamine (3.4 g, 30 mmol), K₃PO₄ (8.5 g, 40 mmol), and 1,4-dioxane (10 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-149) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.6 g in 35% yield.

FD-MS C₅₄H₃₁N₃O₂: theoretical value 753, observed value 753

Synthesis Example 1-17

Synthesis of Compound 1-163

[Chem 179]

50

Compound A-28 (3.5 g, 7.9 mmol), carbazole (2.7 g, 16 mmol), CuI (1.5 g, 7.9 mmol), transcyclohexane 1,2-diamine (2.7 g, 23.7 mmol), $\rm K_3PO_4$ (6.7 g, 31.6 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged $_{\rm 40}$ into the funnel. Then, the mixture was extracted with CH $_2$ Cl $_2$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-163) was obtained. The powder was $_{\rm 45}$ purified by sublimation, whereby a white solid was obtained in an amount of 2.2 g in 45% yield.

FD-MS $C_{42}H_{24}N_2S_2$: theoretical value 620, observed value 620

Synthesis Example 1-18

Synthesis of Compound 1-169

[Chem 181]

-continued

Compound A-29 (3.5 g, 7.9 mmol), carbazole (2.7 g, 16 mmol), CuI (1.5 g, 7.9 mmol), transcyclohexane 1,2-diamine (2.7 g, 23.7 mmol), $\rm K_3PO_4$ (6.7 g, 31.6 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-169) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.3 g in 47% yield.

FD-MS $\rm C_{42}H_{24}N_2S_2;$ theoretical value 620, observed value 620

Synthesis Example 1-19

Synthesis of Compound 1-191

(1) Synthesis of Compound A-28

25

1,4-dibromo-2,5-dimethoxybenzene (4.4 g, 15.0 mmol), Compound A-27 (11.0 g, 36.0 mmol), and a 2 M aqueous solution of Na₂CO₃ (30 mL, 60.0 mmol), DME (30 mL), toluene (30 mL), and Pd[PPh₃]₄ (0.87 g, 0.75 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (150 mL) was charged 20 into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 9.5 g in 97% yield.

FD-MS C₄₄H₃₀F₂N₂O₂: theoretical value 656, observed value 656 [Chem 183]

(2) Synthesis of Compound A-29

[Chem 184] $1M\;\mathrm{BBr_3}$ CH₂Cl₂ A-29

Compound A-28 (9.5 g, 14.5 mmol), a 1-M solution of BBr₃ in CH₂Cl₂ (90 mL, 90.0 mmol), and CH₂Cl₂ (100 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO3. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified 65 by column chromatography, whereby a white solid was obtained in an amount of 8.0 g in 88% yield.

FD-MS C₄₂H₂₆F₂N₂O₂: theoretical value 628, observed value 628 [Chem 185]

(3) Synthesis of Compound 1-191

[Chem 186]

$$K_2CO_3$$
 N
 F
 N
 $A-29$

1-191

Compound A-29 (8.0 g, 12.7 mmol), K₂CO₃ (7.0 g, 50.9 mmol), and NMP (240 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 200° C. for 3 hours.

After the completion of the reaction, the resultant was cooled to room temperature. Toluene (500 mL) was charged into the resultant sample. The mixture was transferred to a separating funnel, and was washed with water. The washed product was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 1-191) was obtained. The powder was purified by sublimation, whereby a white solid was

10

60

obtained in an amount of 2.4 g in 31% yield. FD-MS C₄₂H₂₄N₂O₂: theoretical value 588, observed ⁵

An apparatus and measurement conditions adopted for field desorption mass spectrometry (FD-MS) in each of Synthesis Examples 1-1 to 1-19 are shown below.

Apparatus: HX110 (manufactured by JEOL Ltd.) Conditions: accelerating voltage 8 kV scan range m/z=50 to 1,500 emitter kind: carbon emitter current: 0 mA→2 mA/min→40 mA (held for 10

Example 1-1

(Production of Organic EL Device)

value 588

minutes)

A glass substrate provided with an ITO transparent elec- 20 trode measuring 25 mm by 75 mm by 1.1 mm (manufactured by GEOMATEC Co., Ltd.) was subjected to ultrasonic cleaning in isopropyl alcohol for 5 minutes. Further, the substrate was subjected to ultraviolet (UV)-ozone cleaning for 30 minutes.

The glass substrate provided with a transparent electrode thus cleaned was mounted on a substrate holder of a vacuum deposition apparatus. First, Compound 1-A was deposited from the vapor onto the surface of the glass substrate on the side where a transparent electrode line was formed so as to $\,^{30}$ cover the transparent electrode, whereby a hole transporting layer having a thickness of 30 nm was obtained.

Compound 1-1 as a host for phosphorescence and Ir(Phppy)3 as a dopant for phosphorescence were co-deposited from the vapor onto the hole transporting layer, whereby a 35 phosphorescent layer having a thickness of 30 nm was obtained. The concentration of Ir(Ph-ppy)₃ was 5 masse.

Subsequently, Compound 1-B having a thickness of 10 nm, Compound 1-C having a thickness of 20 nm, LiF having a thickness of 1 nm, and metal Al having a thickness of 80 nm 40 were sequentially laminated on the phosphorescent layer, whereby a cathode was obtained. It should be noted that LiF as an electron injectable electrode was formed at a rate of 1 Å/min.

[Chem 187]

-continued

Compound 1-B

Compound 1-C

Ir(Ph-ppy)3(facial body)

(Evaluation of Organic EL Device for Light Emitting Performance)

The organic EL device thus produced was caused to emit light by being driven with a direct current. The luminance (L) of the emitted light and the current density at which the device started to emit the light were measured. Then, the current efficiency (L/J) of the device at a luminance of 1,000 cd/m² was determined. Further, the lifetime of the device at a luminance of 20,000 cd/m² was determined. Table 1 shows the results.

Examples 1-2 to 1-19

Organic EL devices were each produced in the same manner as in Example 1-1 except that a host material listed in Table 1 was used instead of Host Compound 1-1 in Example 1-1, and the devices were each evaluated in the same manner as in Example 1-1. Table 1 shows the results of the evaluation for light emitting performance.

(1-a)

(1-b)

Organic EL devices were each produced in the same manner as in Example 1-1 except that the following compounds (1-a) to (1-c) described in EP 0908787 A was used as a host material instead of Host Compound 1-1 in Example 1-1, and the devices were each evaluated in the same manner as in Example 1-1. Table 1 shows the results of the evaluation for light emitting performance.

Organic EL devices were each produced in the same manner as in Example 1 except that the following compounds (1-d) to (1-i) described in WO 2006-122630 was used as a 20 host material instead of Host Compound 1-1 in Example 1-1, and the devices were each evaluated in the same manner as in Example 1-1. Table 1 shows the results of the evaluation for light emitting performance.

Comparative Examples 1-10 and 1-11

An organic EL device was produced in the same manner as in Example 1-1 except that the following compound (1-j) or ³⁰ (1-k) described in WO 2007-063754 was used as a host material instead of Host Compound 1-1 in Example 1-1, and the device was evaluated in the same manner as in Example 1-1. Table 1 shows the results of the evaluation for light emitting performance.

(1-h)

(1-j)

15

-continued

TABLE 1

25		Host compound	Voltage (V) @20 mA/ cm ²	Efficiency (cd/A) @1,000 cd/m ²	Life time (hr) @20,000 cd/m ²
	Example 1-1	(1-1)	4.8	58.1	400
	Example 1-2	(1-17)	4.9	60.9	390
	Example 1-3	(1-18)	5.0	60.2	400
30	Example 1-4	(1-34)	4.8	57.4	450
20	Example 1-5	(1-46)	4.6	58.3	500
	Example 1-6	(1-49)	4.7	57.8	500
	Example 1-7	(1-68)	4.8	60.7	300
35	Example 1-8	(1-74)	5.0	62.9	300
	Example 1-9	(1-85)	5.0	63.3	300
33	Example 1-10	(1-87)	5.1	63.3	350
	Example 1-11	(1-113)	4.8	62.1	300
	Example 1-12	(1-116)	4.6	59.9	300
	Example 1-13	(1-138)	4.5	42.2	170
	Example 1-14	(1-140)	4.7	61.6	360
40	Example 1-15	(1-148)	4.9	41.5	140
	Example 1-16	(1-149)	5.0	41.8	140
	Example 1-17	(1-163)	4.7	60.4	300
	Example 1-18	(1-169)	4.7	60.6	280
	Example 1-19	(1-191)	5.0	60.2	520
45	Comparative	(1-a)	4.6	26.5	50
	Example 1-1				
	Comparative	(1-b)	4.7	26.1	30
	Example 1-2				
50	Comparative	(1-c)	4.2	17.6	30
	Example 1-3				
	Comparative	(1-d)	4.9	36.3	20
	Example 1-4				
	Comparative	(1-e)	4.3	27.4	40
	Example 1-5				
55	Comparative	(1-f)	5.6	35.9	120
33	Example 1-6				
	Comparative	(1-g)	5.6	36.1	100
	Example 1-7				
60	Comparative	(1-h)	4.8	38.5	10
	Example 1-8				
	Comparative	(1-i)	4.9	39.6	10
	Example 1-9				
	Comparative	(1-j)	4.3	17.3	30
	Example 1-10				
	Comparative	(1-k)	4.5	17.9	20
65	Example 1-11				

[Chem 191]

Synthesis of Compound 2-1

(1) Synthesis of Compound B-1

1,3-dibromo-4,6-diffuorobenzene (50.0 g, 183.9 mmol), 25 2-methoxyphenylboronic acid (67.1 g, 441.4 mmol), and a 2 M aqueous solution of $\rm Na_2CO_3$ (368 mL, 736 mmol), DME (370 mL), toluene (370 mL), and $\rm Pd[PPh_3]_4$ (21.3 g, 18.4 mmol) were loaded in to a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (500 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 40.2 g in 67% yield.

FD-MS $C_{20}H_{16}F_2O_2$: theoretical value 326, observed value 326

(2) Synthesis of Compound B-2

[Chem 190]

Compound B-1 (40.0 g, 122.6 mmol), NBS (43.6 g, 245 mmol) and DMF $(1,100\,\mathrm{mL})$ were loaded into a three-necked

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flask, and the mixture was stirred under an Ar atmosphere at room temperature for 8 hours. After the completion of the reaction, the resultant sample was transferred to a separating funnel, and water (1,000 mL) was charged into the funnel. Then, the mixture was extracted with AcOEt. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 42.1 g in 71% yield.

FD-MS $\rm C_{20}H_{14}Br_2F_2O_2$: theoretical value 484, observed value 484

(3) Synthesis of Compound B-3

Compound B-2 (40.0 g, 82.6 mmol), a 1-M solution of BBr₃ in CH₂Cl₂ (194 mL, 194 mmol), and CH₂Cl₂ (500 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO₃. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 30.2 g in 80% yield.

B-3

FD-MS $C_{18}H_{10}Br_2F_2O_2$: theoretical value 456, observed value 456

(4) Synthesis of Compound B-4

Compound B-3 (30.0 g, 65.7 mmol), $\rm K_2CO_3$ (19.9 g, 144.5 mmol), and NMP (270 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 150° C. for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (500 mL) was charged into the funnel. Then, the mixture was extracted with AcOEt. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 21.9 g in 80% yield.

FD-MS $C_{18}H_8Br_2O_2$: theoretical value 416, observed value 416

(5) Synthesis of Compound 2-1

[Chem 193]

Compound B-4 (3 g, 7.2 mmol), carbazole (2.9 g, 17.3 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), $\rm K_3PO_4$ (6.1 g, 28.8 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was trans-

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ferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-1) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.5 g in 60% yield.

FD-MS $\rm C_{42}H_{24}N_2O_2$: theoretical value 588, observed value 588

Synthesis Example 2-2

Synthesis of Compound 2-17

(1) Synthesis of Compound B-5

[Chem 194]

35

O B-5

CuI.

Compound B-4 (3 g, 7.2 mmol), carbazole (1.5 g, 7.2 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), $\rm K_3PO_4$ (6.1 g, 28.8 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 2.0 g in 54% yield.

FD-MS $\rm C_{30}\rm H_{16} Br NO_2$: theoretical value 502, observed value 502

(2) Synthesis of Compound 2-17

FD-MS $\rm C_{54}H_{32}N_2O_4$: theoretical value 740, observed value 740

Synthesis Example 2-3

Synthesis of Compound 2-18

Compound B-5 (3.0 g, 6.0 mmol), Compound B-6 (2.4 g, 6.6 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and $\rm Pd[PPh_3]_4$ (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-17) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.5 g in 56% yield.

Compound B-5 (3.0 g, 6.0 mmol), Compound B-7 (1.7 g, 6.0 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh₃]₄ (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

2-18

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-18) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.1 g in 52% yield.

FD-MS $C_{48}H_{27}NO_3$: theoretical value 665, observed value 665

15

50

Synthesis of Compound 2-34

(1) Synthesis of Compound B-8

[Chem 197]

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

Compound (2-1) (10 g, 17 mmol) and $\rm CH_2Cl_2$ (100 mL) were loaded into a three-necked flask and bromine (5.4 g, 34 mmol) was dropped thereto under an Ar atmosphere at 0° C. After that, the mixture was stirred at room temperature for 8 hours. After the completion of the reaction, the sample was transferred to a separating funnel and water (50 mL) was added thereto, followed by extraction with $\rm CH_2Cl_2$. An 40 organic layer was washed with a saturated NaNO2 aqueous solution (50 mL) and dried with MgSO4, followed by filtration and concentration. The sample was purified by a column chromatography, whereby a white solid was obtained in an amount of 7.6 g in 60% yield.

FD-MS $\rm C_{42}H_{22}Br_2N_2O_2$: theoretical value 746, observed value 746

(2) Synthesis of Compound 2-34

Compound B-8 (3.7 g, 4.9 mmol), phenylboronic acid (1.32 g, 10.8 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (5 mL, 9.8 mmol), DME (10 mL), toluene (10 mL), and Pd[PPh₃]₄ (0.29 g, 0.25 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-34) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.5 g in 40% yield.

FD-MS $\rm C_{54}H_{32}N_2O_2;$ theoretical value 740, observed value 740

Synthesis Example 2-5

Synthesis of Compound 2-46

(1) Synthesis of Compound B-9

Compound B-5 (10 g, 20 mmol) and THF (200 mL) were $\,$ 15 loaded into a three-necked flask, and the mixture was cooled to -78° C. Then, n-BuLi (1.65-M solution in n-hexane, 13.3 mL, 22 mmol) was added dropwise to the flask, and the resultant mixture was stirred at -78° C. for 20 minutes. Triisopropyl boronate (11.3 g, $60\,\text{mmol}$) was added to the result- 20ant, and the mixture was stirred at -78° C. for 1 hour. After that, the resultant was left to stand overnight at room temperature. Then, 1N HCl (40 mL) was charged into the resultant, and the mixture was stirred at room temperature for 1 hour. The resultant sample was concentrated, and was then 25 transferred to a separating funnel. Water (50 mL) was charged into the funnel, and the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by recrystallization (toluene-hexane), whereby a white solid was 30 obtained in an amount of 5.9 g in 63% yield.

(2) Synthesis of Compound 2-46

Compound B-5 (3.0 g, 6.0 mmol), Compound B-9 (3.1 g, 6.6 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and $\rm Pd[PPh_3]_4$ (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-46) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.1 g in 41% yield.

FD-MS $\rm C_{60}H_{32}N_2O_4\!:$ theoretical value 844, observed value 844

Synthesis of Compound 2-49

[Chem 201]

55

Compound B-9 (10.2 g, 21.9 mmol), 1,3,5-tribromobenzene (2.3 g, 7.3 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (22.5 mL, 45 mmol), DME (15 mL), toluene (15 mL), and $\rm Pd[PPh_3]_4$ (0.63 g, 0.56 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with $\mathrm{MgSO_4}$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-49) was obtained. The powder 65 was purified by sublimation, whereby a white solid was obtained in an amount of 1.4 g in 14% yield.

FD-MS $C_{96}H_{51}N_3O_6{:}$ theoretical value 1,342, observed $^{50}\,$ value 1,342

Synthesis Example 2-7

Synthesis of Compound 2-68

Compound B-10 (3 g, 7.2 mmol), carbazole (3.0 g, 14.4 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), $\rm K_3PO_4$ (6.1 g, 28.8 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-68) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.9 g in 46% yield.

FD-MS $\rm C_{42}H_{24}N_2O_2;$ theoretical value 588, observed value 588

Synthesis Example 2-8

Synthesis of Compound 2-74

518

Compound B-11 (3.0 g, 6.0 mmol), Compound B-6 (2.4 g, 6.6 mmol), a 2 M aqueous solution of $\mathrm{Na_2CO_3}$ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh_3]_4 (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

2-74

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-74) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.8 g in 40% yield.

FD-MS $\rm C_{54}H_{32}N_2O_2;$ theoretical value 740, observed value 740

Synthesis Example 2-9

Synthesis of Compound 2-85

[Chem 203]

B-11

³ [Chem 204]

B-11

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Compound B-11 (3.0 g, 6.0 mmol), Compound B-7 (1.9 g, 6.6 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh_3]_4 (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-85) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.1 g in 52% yield.

FD-MS $\rm C_{48}H_{27}NO_3$: theoretical value 665, observed value 665

Synthesis Example 2-10

Synthesis of Compound 2-87

Compound B-12 (3.3 g, 5.0 mmol), phenylboronic acid (0.67 g, 5.5 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (5 mL, 10 mmol), DME (10 mL), toluene (10 mL), and $\rm Pd[PPh_3]_4$ (0.29 g, 0.25 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-87) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.3 g in 40% yield.

FD-MS $\rm C_{48}\rm H_{28}\rm N_2\rm O_2$: theoretical value 664, observed value 664

Synthesis Example 2-11

Synthesis of Compound 2-113

(1) Synthesis of Compound B-13

Compound B-11 (10 g, 20 mmol) and THF (200 mL) were loaded into a three-necked flask, and the mixture was cooled to -78° C. Then, n-BuLi (1.65-M solution in n-hexane, 13.3 mL, 22 mmol) was added dropwise to the flask, and the 15 resultant mixture was stirred at -78° C. for 20 minutes. Triisopropyl boronate (11.3 g, 60 mmol) was added to the resultant, and the mixture was stirred at -78° C. for 1 hour. After that, the resultant was left to stand overnight at room temperature. Then, 1N HCl (40 mL) was charged into the result- 20 ant, and the mixture was stirred at room temperature for 1 hour. The resultant sample was concentrated, and was then transferred to a separating funnel. Water (50 mL) was charged into the funnel, and the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by recrystallization (toluene-hexane), whereby a white solid was obtained in an amount of 6.3 g in 670 yield.

(2) Synthesis of Compound 2-113

[Chem 207]

Compound B-11 (3.0 g, 6.0 mmol), Compound B-13 (3.1 g, 6.6 mmol), a 2 M aqueous solution of Na₂CO₃ (6.0 mL, 12 mmol), DME (12 mL), toluene (12 mL), and $Pd[PPh_3]_4\,(0.35$ g, 0.30 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 113) was obtained. The powder was purified by sublimation, whereby a white solid was 25 obtained in an amount of 2.7 g in 53% yield.

FD-MS C₆₀H₃₂N₂O₄: theoretical value 844, observed value 844

Synthesis Example 2-12

Synthesis of Compound 2-116

[Chem 208]

2-116

Compound B-13 (10.2 g, 21.9 mmol), 1,3,5-tribromobenzene (2.3 g, 7.3 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (22.5 mL, 45 mmol), DME (15 mL), toluene (15 mL), and 50 Pd[PPh₃]₄ (0.63 g, 0.56 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-116) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.7 g in 17% yield.

FD-MS $C_{96}H_{51}N_3O_6$: theoretical value 1,342, observed value 1,342

Synthesis Example 2-13

Synthesis of Compound 2-138

(1) Synthesis of Compound B-15

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-continued

$$\begin{array}{c|c} & & & 10 \\ \hline \\ & N \\ & N \\ \hline \\ N \\ & N \\ & 15 \\ \hline \\ & 15 \\ \hline \\ & B-15 \\ \end{array}$$

Compound B-14 (24.6 g, 74 mmol), 1,3-dibromo-4,6-difluorobenzene (20 g, 74 mmol), and a 2 M aqueous solution of Na $_2$ CO $_3$ (75 mL, 150 mmol), DME (150 mL), toluene (150 mL), and Pd[PPh $_3$] $_4$ (4.3 g, 3.7 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with $\rm CH_2Cl_2$. The extract was dried with MgSO_4, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 20 g in 56% yield.

FD-MS $\rm C_{24}H_{13}BrF_2N_2O_2$: theoretical value 479, observed value 479

(2) Synthesis of Compound B-17

-continued

Compound B-15 (20.0 g, 42 mmol), Compound B-16 (14.6 g, 46 mmol), and a 2 M aqueous solution of Na₂CO₃ (42 mL, 84 mmol), DME (85 mL), toluene (85 mL), and Pd[PPh₃]₄ (2.4 g, 2.1 mmol) were loaded into a three-necked flask, and 35 the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water ($100\,\mathrm{mL}$) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 13.3 g in 47% yield.

5 FD-MS $C_{43}H_{27}F_2N_3O_3$: theoretical value 671, observed value 671

(3) Synthesis of Compound B-18

 $1M \; \mathrm{BBr}_3$

CH₂Cl₂

[Chem 210]

$$O_{2N}$$
 F B -15

[Chem 211]
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B-17

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Compound B-17 (13.0 g, 19.4 mmol), a 1-M solution of 15 BBr₃ in CH₂Cl₂ (100 mL, 100 mmol), and CH₂Cl₂ (200 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO₃. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 10.6 g in 83% yield.

FD-MS C₄₂H₂₅F₂N₃O₃: theoretical value 657, observed value 657

(4) Synthesis of Compound B-19

[Chem 212]

Compound B-18 (10.0 g, 15.2 mmol), 5% Ru—C (0.61 g), and ethanol (57 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 70° C. Hydrazine monohydrate (4.6 g, 91.9 mmol) was dissolved in ethanol (5 mL) and dropped thereto. After that, the reaction mixture was refluxed for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The 65 sample was filtrated under reduced pressure, and the filtrate was concentrated. The sample was purified by silica gel col-

umn chromatography, whereby a white solid was obtained in an amount of 8.0 g in 84% yield.

FD-MS C₄₂H₂₇F₂N₃O: theoretical value 627, observed value 627

(5) Synthesis of Compound B-20

[Chem 213]

$$K_2CO_3$$
 NMP
 H_2N
 F
 $B-19$
 $B-20$

Compound B-19 (8.0 g, 12.7 mmol), K₂CO₃ (3.9 g, 28.1 mmol), and NMP (50 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 150° C. for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 6.0 g in 80% yield.

FD-MS $C_{42}H_{25}N_3O$: theoretical value 587, observed value 587

(6) Synthesis of Compound 2-138

[Chem 214]

Compound B-20 (5.0 g, 8.5 mmol), iodobenzene (1.7 g, 8.5 mmol), CuI (1.6 g, 8.5 mmol), transcyclohexane 1,2-diamine (2.9 g, 25.5 mmol), $\rm K_3PO_4$ (7.2 g, 34 mmol), and 1,4-dioxane (9 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\rm CH_2Cl_2$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-138) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.7 g in 47% yield.

FD-MS $\rm C_{48}H_{29}N_{30}$: theoretical value 663, observed value 663

Synthesis Example 2-14

Synthesis of Compound 2-140

Compound B-21 (2.8 g, 7.3 mmol), carbazole (2.4 g, 14.6 mmol), CuI (1.4 g, 7.3 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.9 mmol), $\rm K_3PO_4$ (6.2 g, 29.2 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-140) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.4 g in 55% yield.

FD-MS $\rm C_{42}H_{24}N_2OS:$ theoretical value 604, observed value 604

Synthesis Example 2-15

Synthesis of Compound 2-148

(1) Synthesis of Compound B-23

Compound B-22 (5.0 g, 8.5 mmol), 2-bromodibenzofuran (2.1 g, 8.5 mmol), CuI (1.6 g, 8.5 mmol), transcyclohexane 1,2-diamine (2.9 g, 25.5 mmol), K₃PO₄ (7.2 g, 34 mmol), and 1,4-dioxane (9 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 25

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 2.9 g in 45% yield.

752

FD-MS $C_{54}H_{32}N_{40}$: theoretical value 752, observed value $_{35}$ (2) Synthesis of Compound 2-148 40 [Chem 217] 45

Compound B-23 (2.9 g, 3.9 mmol), iodobenzene (0.8 g, 3.9 mmol), CuI (0.74 g, 3.9 mmol), transcyclohexane 1,2-diamine (1.3 g, 11.7 mmol), K₃PO₄ (3.3 g, 15.6 mmol), and 1,4-dioxane (4 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and 50 mL of water was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-148) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.4 g in 43% yield.

FD-MS $\mathrm{C}_{60}\mathrm{H}_{36}\mathrm{N}_{40}\!:$ theoretical value 828, observed value 828

Synthesis Example 2-16

Synthesis of Compound 2-149

Dioxane, reflux

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Compound B-24 (4.2 g, 10 mmol), 2-bromodibenzofuran (5.0 g, 20 mmol), CuI (1.9 g, 10 mmol), transcyclohexane 1,2-diamine (3.4 g, 30 mmol), K₃PO₄ (8.5 g, 40 mmol), and 1,4-dioxane (10 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged $\,^{30}$ into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-149) was obtained. The powder was 35 purified by sublimation, whereby a white solid was obtained in an amount of 2.1 g in 28% yield.

FD-MS $C_{54}H_{31}N_3O_2$: theoretical value 753, observed value 753

Synthesis Example 2-17

Synthesis of Compounds 2-157 and 2-163

(1) Synthesis of Compound B-26

Compound B-25 (29.1 g, 66 mmol), 1,3-dibromobenzene (7.1 g, 30 mmol), a 2 M aqueous solution of Na₂CO₃ (60 mL, 120 mmol), DME (60 mL), toluene (60 mL), and Pd[PPh₃]₄ (1.7 g, 1.5 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with $MgSO_4$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 9.1 g in 43% yield.

FD-MS $C_{48}H_{36}N_2O_4$: theoretical value 704, observed value 704

(2) Synthesis of Compound B-27

Compound B-26 (9.0 g, 12.8 mmol) and THF (45 mL) were loaded into a three-necked flask, and the mixture was stirred at 0° C. MeMgBr (0.97M THF solution, 59 mL, 57

B-27

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535 mmol) was dropped thereto. After stirred at 0° C. for 3 hours,

2-157 and 2-163) was obtained. The obtained powder was purified by sublimation, whereby a white solid was obtained. The obtained amount and yield of Compound 2-157 were 2.4 g and 51%, respectively. The obtained amount and yield of Compound 2-163 were 1.2 g and 25%, respectively.

536

FD-MS $C_{48}H_{36}N_2$: theoretical value 640, observed value 640 for both of Compounds (2-157 and 2-163)

Synthesis Example 2-18

Synthesis of Compound 2-169

the mixture was left to stand at room temperature overnight. The sample was transferred to a separating funnel, and a saturated NH₄Cl aqueous solution (50 mL) was added, followed by extraction with AcOEt. The sample was dried with MgSO₄, followed by filtration and concentration. The sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 6.9 g in 80% yield.

FD-MS C₄₈H₄₀N₂O₂: theoretical value 676, observed value 676

(3) Synthesis of Compounds 2-157 and 2-163

[Chem 221] PPA НО B-27 35 2-157 2-163

Compound B-27 (5 g, 7.4 mmol) and polyphosphoric acid (10 g) were loaded into a three-necked flask, and the mixture was stirred at 40° C. for 8 hours.

After the completion of the reaction, the mixture was 60 cooled to room temperature. The sample was dissolved in water (100 mL) and CH₂Cl₂ (100 mL) and transferred to a separating funnel, followed by extraction with CH₂Cl₂. The resultant was dried with MgSO₄, followed by filtration and concentration. The sample was purified by silica gel chroma- 65 tography. After concentration to dryness, recrystallization was carried out twice, whereby a white powder (Compounds

Compound B-28 (3.5 g, 7.9 mmol), carbazole (2.7 g, 16 mmol), CuI (1.5 g, 7.9 mmol), transcyclohexane 1,2-diamine (2.7 g, 23.7 mmol), K_3PO_4 (6.7 g, 31.6 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the $mixture \ was \ refluxed \ under \ an \ argon \ atmosphere \ for \ 10 \ hours.$

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and 50 mL of water was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 2-169) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.9 g in 40% yield.

FD-MS C₄₂H₂₄N₂S₂: theoretical value 620, observed

An apparatus and measurement conditions adopted for field desorption mass spectrometry (FD-MS) in each of Synthesis Examples 2-1 to 2-18 are shown below.

Apparatus: HX110 (manufactured by JEOL Ltd.)

Conditions: accelerating voltage 8 kV

scan range m/z=50 to 1,500

emitter kind: carbon

emitter current: 0 mA→2 mA/min→40 mA (held for 10 minutes)

Example 2-

(Production of Organic EL Device)

A glass substrate provided with an ITO transparent electrode measuring 25 mm by 75 mm by 1.1 mm (manufactured by GEOMATEC Co., Ltd.) was subjected to ultrasonic cleaning in isopropyl alcohol for 5 minutes. Further, the substrate was subjected to ultraviolet (UV)-ozone cleaning for 30 minutes.

The glass substrate provided with a transparent electrode thus cleaned was mounted on a substrate holder of a vacuum deposition apparatus. First, Compound 2-A was deposited from the vapor onto the surface of the glass substrate on the side where a transparent electrode line was formed so as to cover the transparent electrode, whereby a hole transporting layer having a thickness of 30 nm was obtained.

Compound 2-1 as a host for phosphorescence and Ir(Ph-ppy)3 as a dopant for phosphorescence were co-deposited from the vapor onto the hole transporting layer, whereby a phosphorescent layer having a thickness of 30 nm was obtained. The concentration of Ir(Ph-ppy)3 was 5 mass %.

Subsequently, Compound 2-B having a thickness of 10 nm, Compound 2-C having a thickness of 20 nm, LiF having a thickness of 1 nm, and metal Al having a thickness of 80 nm were sequentially laminated on the phosphorescent layer, whereby a cathode was obtained. It should be noted that LiF as an electron injectable electrode was formed at a rate of 1 Å/min.

[Chem 223]

Ir(Ph-ppy)3(facial body)

(Evaluation of Organic EL Device for Light Emitting Performance)

The organic EL device thus produced was caused to emit light by being driven with a direct current. The luminance (L) of the emitted light and the current density at which the device started to emit the light were measured. Then, the current efficiency (L/J) of the device at a luminance of 1,000 cd/m 2 was determined. Further, the lifetime of the device at a luminance of 20,000 cd/m 2 was determined. Table 2 shows the results.

Examples 2-2 to 2-19

Organic EL devices were each produced in the same manner as in Example 2-1 except that a host material listed in Table 2 was used instead of Host Compound 2-1 in Example 2-1, and the devices were each evaluated in the same manner as in Example 2-1. Table 2 shows the results of the evaluation for light emitting performance.

Comparative Examples 2-1 to 2-3

Organic EL devices were each produced in the same manner as in Example 2-1 except that the following compounds (2-a) to (2-c) described in EP 0908787 A was used as a host material instead of Host Compound 2-1 in Example 2-1, and the devices were each evaluated in the same manner as in Example 2-1. Table 2 shows the results of the evaluation for light emitting performance.

Comparative Examples 2-4 to 2-9

Organic EL devices were each produced in the same man-65 ner as in Example 2-1 except that the following compounds (2-d) to (2-i) described in WO 2006-122630 was used as a host material instead of Host Compound 2-1 in Example 2-1,

Compound 2-C

(2-c) 45

and the devices were each evaluated in the same manner as in Example 2-1. Table 2 shows the results of the evaluation for light emitting performance.

Comparative Examples 2-10 and 2-11

An organic EL device was produced in the same manner as in Example 2-1 except that the following compound (2-j) or (2-k) described in WO 2007-063754 was used as a host material instead of Host Compound 2-1 in Example 2-1, and the device was evaluated in the same manner as in Example 2-1. Table 1 shows the results of the evaluation for light emitting performance.

-continued

541 -continued			
(2-h)	5		Host comp
$\begin{array}{c} \\ \\ \\ \\ \\ \end{array}$	10	Example 2-1 Example 2-2 Example 2-3 Example 2-4 Example 2-5 Example 2-6	(2-1) (2-17) (2-18) (2-34) (2-46) (2-49)
	15	Example 2-7 Example 2-8 Example 2-9 Example 2-10 Example 2-11 Example 2-12	(2-68) (2-74) (2-85) (2-87) (2-11) (2-11)
	20	Example 2-13 Example 2-14 Example 2-15 Example 2-16 Example 2-17	(2-13) (2-14) (2-14) (2-14) (2-15)
N	25	Example 2-18 Example 2-19 Comparative Example 2-1	(2-16) (2-16) (2-a)
	30	Comparative Example 2-2 Comparative Example 2-3	(2-b) (2-c)
(2-j)		Comparative Example 2-4 Comparative	(2-d) (2-e)

Synthesis Example 3-1

Synthesis of Compound 3-1

(1) Synthesis of Compound C-1

-continued

1,2-dibromo-3,6-difluorobenzene (50.0 g, 183.9 mmol), 2-methoxyphenylboronic acid (67.1 g, 441.4 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (368 mL, 736 mmol), DME (370 mL), toluene (370 mL), and Pd[PPh_3]_4 (21.3 g, 18.4 mmol) 15 were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (500 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained 25 in an amount of 30.6 g in 51% yield.

FD-MS $C_{20}H_{16}F_2O_2$: theoretical value 326, observed value 326

(2) Synthesis of Compound C-2

[Chem 226]

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Compound C-1 (30.0 g, 91.9 mmol), NBS (32.8 g, 184 mmol), and DMF (820 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at room temperature for 8 hours. After the completion of the reaction, the resultant sample was transferred to a separating funnel, and water (1,000 mL) was charged into the funnel. Then, the mixture was extracted with AcOEt. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 32 g in 72% yield.

FD-MS $C_{20}H_{14}Br_2F_2O_2$: theoretical value 484, observed value 484

(3) Synthesis of Compound C-3

Compound C-2 (32.0 g, 66.1 mmol), a 1-M solution of BBr₃ in CH₂Cl₂ (155 mL, 155 mmol), and CH₂Cl₂ (430 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO₃. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 24.1 g in 80% yield.

FD-MS $\rm C_{18}H_{10}Br_2F_2O_2$: theoretical value 456, observed value 456

(4) Synthesis of Compound C-4

Compound C-3 (24.1 g, 52.8 mmol), K_2CO_3 (16.0 g, 116 mmol), and NMP (220 mL) were loaded into a three-necked

flask, and the mixture was stirred under an Ar atmosphere at 150° C. for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (500 mL) was charged into the funnel. Then, the mixture was extracted with AcOEt. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 18.7 g in 85% yield.

FD-MS $C_{18}H_8Br_2O_2$: theoretical value 416, observed value 416

(5) Synthesis of Compound 3-1

546

ness, and was then recrystallized twice, whereby a white powder (Compound 3-1) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.7 g in 39% yield.

FD-MS $C_{42}H_{24}N_2O_2$: theoretical value 588, observed value 588

Synthesis Example 3-2

Synthesis of Compound 3-17

(1) Synthesis of Compound C-5

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Compound C-4 (3 g, 7.2 mmol), carbazole (2.9 g, 17.3 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), $\rm K_3PO_4$ (6.1 g, 28.8 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the $\rm _{60}$ mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. 65 The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dry-

Compound C-4 (3 g, 7.2 mmol), carbazole (1.5 g, 7.2 mmol), CuI (1.4 g, 7.2 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.6 mmol), $\rm K_3PO_4$ (6.1 g, 28.8 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 2.2 g in 60% yield.

FD-MS C₃₀H₁₆BrNO₂: theoretical value 502, observed value 502

(2) Synthesis of Compound 3-17

Compound C-5 (3.0 g, 6.0 mmol), Compound C-6 (2.4 g, 6.6 mmol), a 2 M aqueous solution of Na₂CO₃ (6 mL, 12 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh₃]₄ (0.35 g, 0.3 mmol) were loaded into a three-necked flask, and the 60 mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. 65 The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel

column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-17) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.3 g in 30% yield.

FD-MS $C_{54}H_{30}N_2O_2$: theoretical value 740, observed value 740

Synthesis Example 3-3

Synthesis of Compound 3-18

Compound C-5 (3.3 g, 6.6 mmol), Compound C-7 (2.1 g, 7.3 mmol), a 2 M aqueous solution of Na₂CO₃ (6 mL, 13 mmol), DME (13 mL), toluene (1 mL), and Pd[PPh₃]₄ (0.38 g, 0.33 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged

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into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with $\mathrm{MgSO_4}$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-18) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.4 g in 31% yield.

FD-MS $\mathrm{C_{48}H_{27}NO_3}$: theoretical value 665, observed value $_{10}$

Synthesis Example 3-4

Synthesis of Compound 3-34

(1) Synthesis of Compound C-8

Compound (3-1) (10 g, 17 mmol) and CH₂Cl₂ (100 mL) were loaded into a three-necked flask and bromine (5.4 g, 34 mmol) was dropped thereto under an Ar atmosphere at 0° C. After that, the mixture was stirred at room temperature for 8 hours. After the completion of the reaction, the sample was transferred to a separating funnel and water (50 mL) was added thereto, followed by extraction with CH₂Cl₂. An organic layer was washed with a saturated NaNO₂ aqueous solution (50 mL) and dried with MgSO₄, followed by filtration and concentration. The sample was purified by a column 65 chromatography, whereby a white solid was obtained in an amount of 3.7 g in 29% yield.

C-8

FD-MS $\rm C_{42}H_{22}Br_2N_2O_2$: theoretical value 746, observed value 746

(2) Synthesis of Compound 3-34

Compound C-8 (3.7 g, 4.9 mmol), phenylboronic acid (1.32 g, 10.8 mmol), a 2 M aqueous solution of $\mathrm{Na_2CO_3}$ (5 mL, 9.8 mmol), DME (10 mL), toluene (10 mL), and Pd[PPh_3]_4 (0.29 g, 0.25 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-34) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.2 g in 32% yield.

FD-MS $C_{54}H_{32}N_2O_2$: theoretical value 740, observed value 740

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Synthesis of Compound 3-46

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(2) Synthesis of Compound 3-46

(1) Synthesis of Compound C-9

[Chem 235]

Compound C-5 (10 g, 20 mmol) and THF (200 mL) were loaded into a three-necked flask, and the mixture was cooled $_{50}$ to -78° C. Then, n-BuLi (1.65-M solution in n-hexane, 13.3 mL, 22 mmol) was added dropwise to the flask, and the resultant mixture was stirred at -78° C. for 1 hour. Triisopropyl boronate (11.3 g, 60 mmol) was added to the resultant, and the mixture was stirred at -78° C. for 20 minutes. After that, the resultant was left to stand overnight at room temperature. Then, 1N HCl (40 mL) was charged into the resultant, and the mixture was stirred at room temperature for 1 hour. The resultant sample was concentrated, and was then transferred 60 to a separating funnel. Water (50 mL) was charged into the funnel, and the mixture was extracted with CH2Cl2. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by recrystal- $_{65}$ lization (toluene-hexane), whereby a white solid was obtained in an amount of 5.1 g in 55% yield.

Compound C-5 (3.1 g, 6.2 mmol), Compound C-9 (3.2 g, 6.8 mmol), a 2 M aqueous solution of Na₂CO₃ (6.2 mL, 12.4 mmol), DME (12 mL), toluene (12 mL), and Pd[PPh₃]₄ (0.36 g, 0.31 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

3-46

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-46) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.1 g in 20% yield.

[Chem 238]

FD-MS $\rm C_{60}H_{32}N_2O_4\!:$ theoretical value 844, observed value 844

Synthesis Example 3-6

Synthesis of Compound 3-49

a white powder (Compound 3-49) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.5 g in 15% yield.

FD-MS $C_{96}H_{51}N_3O_6$: theoretical value 1,342, observed value 1,342

Synthesis Example 3-7

Synthesis of Compound 3-71

(1) Synthesis of Compound C-11

+
B(OH)₂
C-10
Br
F
Pd[PPh₃]₄
Na₂CO₃ 2M aq.
DME/Toluene

Br
Pd[PPh₃]₄
Na₂CO₃ 2M aq.
DME/Toluene

Compound C-9 (10.2 g, 21.9 mmol), 1,3,5-tribromobenzene (2.3 g, 7.3 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (22.5 mL, 45 mmol), DME (15 mL), toluene (15 mL), and Pd[PPh₃]₄ (0.63 g, 0.56 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was 60 cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel 65 column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby

Compound C-10 (24.6 g, 74 mmol), 1,2-dibromo-3,6-difluorobenzene (20 g, 74 mmol), a 2 M aqueous solution of $\mathrm{Na_2CO_3}$ (75 mL, 150 mmol), DME (150 mL), toluene (150 mL), and $\mathrm{Pd}[\mathrm{PPh_3}]_4$ (4.3 g, 3.7 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with CH $_2$ Cl $_2$. The extract was dried with MgSO $_4$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 14.3 g in 41% yield.

FD-MS C₂₄H₁₃BrF₂N₂O₂: theoretical value 479, observed value 479

(2) Synthesis of Compound C-13

Compound C-11 (14.0 g, 29.2 mmol), Compound C-12 (10.2 g, 32 mmol), a 2 M aqueous solution of Na₂CO₃ (30 mL, 60 mmol), DME (60 mL), toluene (60 mL), and Pd[PPh₃]₄ (1.7 g, 1.5 mmol) were loaded into a three-necked flask, and 55 the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The extract was dried with MgSO₄, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 6.9 g in 35% yield.

FD-MS C₄₃H₂₇F₂N₃O₂: theoretical value 671, observed value 671

(3) Synthesis of Compound C-14

Compound C-13 (6.9 g, 10.3 mmol), a 1-M solution of BBr₃ in CH₂Cl₂ (50 mL, 50 mmol), and CH₂Cl₂ (100 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 0° C. for 8 hours. After that, the mixture was left to stand at room temperature overnight. After the completion of the reaction, the resultant was neutralized with a saturated aqueous solution of NaHCO₃. The resultant sample was transferred to a separating funnel, and was extracted with CH₂Cl₂. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 5.8 g in 85% yield.

FD-MS $C_{42}H_{25}F_2N_3O_3$: theoretical value 657, observed value 657

(4) Synthesis of Compound C-15

[Chem 241]

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Compound C-15 (4.7 g, 7.5 mmol), $\rm K_2\rm CO_3$ (2.3 g, 16.5 mmol), and NMP (24 mL) were loaded into a three-necked flask, and the mixture was stirred under an Ar atmosphere at 150° C. for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\rm CH_2\rm Cl_2$. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 3.6 g in 81% yield.

FD-MS $C_{42}H_{25}N_3O$: theoretical value 587, observed value 587

(6) Synthesis of Compound (1-71)

Compound C-14 (5.8 g, 8.8 mmol), 5% Ru—C (0.35 g), and ethanol (33 mL) were loaded into a three-necked flask, 20 and the mixture was stirred under an Ar atmosphere at 70° C. Hydrazine monohydrate (2.7 g, 53.2 mmol) was dissolved in ethanol (3 mL) and dropped thereto. After that, the reaction mixture was refluxed for 8 hours. After the completion of the reaction, the resultant was cooled to room temperature. The 25 sample was filtrated under reduced pressure, and the filtrate was concentrated. The sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 4.7 g in 85% yield.

FD-MS $C_{42}H_{27}F_2N_3O$: theoretical value 627, observed 30 value 627

(5) Synthesis of Compound C-16

C-16

Compound C-16 (3.0 g, 5.1 mmol), iodobenzene (1.0 g, 5.1 mmol), CuI (0.96 g, 5.1 mmol), transcyclohexane 1,2-di-60 amine (1.7 g, 15.3 mmol), K_3PO_4 (4.3 g, 20.4 mmol), and 1,4-dioxane (6 mL) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂.

The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-71) was obtained. The powder was purified by sublimation, whereby a white solid was obtained 5 in an amount of 1.7 g in 50% yield.

FD-MS $C_{48}H_{29}N_{30}$: theoretical value 663, observed value 663

Synthesis Example 3-8

Synthesis of Compound 3-73

Compound C-17 (2.8 g, 7.3 mmol), carbazole (2.4 g, 14.6 mmol), CuI (1.4 g, 7.3 mmol), transcyclohexane 1,2-diamine (2.5 g, 21.9 mmol), $\rm K_3PO_4$ (6.2 g, 29.2 mmol), and 1,4-dioxane (8 mL) were loaded into a three-necked flask, and the 55 mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-73) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.4 g in 32% yield.

FD-MS $\rm C_{42}H_{24}N_2OS:$ theoretical value 604, observed value 604

Synthesis Example 3-9

Synthesis of Compound 3-75

(1) Synthesis of Compound C-19

C-19

Compound C-18 (5.0 g, 8.5 mmol), 2-bromodibenzofuran (2.1 g, 8.5 mmol), CuI (1.6 g, 8.5 mmol), transcyclohexane 1,2-diamine (2.9 g, 25.5 mmol), $\rm K_3PO_4$ (7.2 g, 34 mmol), and 1,4-dioxane (9 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with ${\rm CH_2Cl_2}$. The resultant sample was purified by column chromatography, whereby a white solid was obtained in an amount of 3.4 g in 52% yield.

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FD-MS $\rm C_{54}H_{32}N_4O$: theoretical value 752, observed value 752

FD-MS $\mathrm{C}_{60}\mathrm{H}_{36}\mathrm{N}_{4}\mathrm{O}$: theoretical value 828, observed value 828

(2) Synthesis of Compound 3-75

Synthesis Example 3-10

Synthesis of Compound 3-76

C-20

Br

CuI,

NH2

K₃PO₄

Dioxane, reflux

N

N

3-76

Compound C-19 (3.0 g, 4.0 mmol), iodobenzene (0.8 g, 4.0 mmol), CuI (0.77 g, 4.0 mmol), transcyclohexane 1,2-diamine (1.3 g, 12.1 mmol), $\rm K_3PO_4$ (2.4 g, 16.1 mmol), and 1,4-dioxane (4 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and $50\,\mathrm{mL}$ of water was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-75) was obtained. The powder was 65 purified by sublimation, whereby a white solid was obtained in an amount of $1.8~\mathrm{g}$ in 54% yield.

Compound C-20 (4.2 g, 10 mmol), 2-bromodibenzofuran (5.0 g, 20 mmol), CuI (1.9 g, 10 mmol), transcyclohexane 1,2-diamine (3.4 g, 30 mmol), $\rm K_3PO_4$ (8.5 g, 40 mmol), and 1,4-dioxane (10 mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (50 mL) was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-76) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.2 g in 30% yield.

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FD-MS $\rm C_{54}H_{31}N_3O_2;$ theoretical value 753, observed value 753

Synthesis Example 3-11

Synthesis of Compound 3-79

(1) Synthesis of Compound C-22

[Chem 248]

$$C-21$$

Compound C-21 (29.1 g, 66 mmol), 1,2-dibromobenzene (7.1 g, 30 mmol), a 2 M aqueous solution of $\rm Na_2CO_3$ (60 mL, 120 mmol), DME (60 mL), toluene (60 mL), and $\rm Pd[PPh_3]_4$ (1.7 g, 1.5 mmol) were loaded into a three-necked flask, and the mixture was refluxed under an Ar atmosphere for 8 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and water (100 mL) was charged into the funnel. Then, the mixture was extracted with $\mathrm{CH_2Cl_2}$. The extract was dried with $\mathrm{MgSO_4}$, and was then filtrated and concentrated. The resultant sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 7.6 g in 36% yield.

FD-MS $\rm C_{48}\rm H_{36}\rm N_2\rm O_4$: theoretical value 704, observed value 704

5 MeMgBr
THF

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Compound C-22 (7.6 g, 10.8 mmol) and THF (38 mL) were loaded into a three-necked flask, and the mixture was stirred at 0° C. MeMgBr (0.97M THF solution, 50 mL, 49 mmol) was dropped thereto. After stirred at 0° C. for 3 hours, the mixture was left to stand at room temperature overnight. The sample was transferred to a separating funnel, and a saturated NH₄Cl aqueous solution (50 mL) was added, followed by extraction with AcOEt. The sample was dried with MgSO₄, followed by filtration and concentration. The sample was purified by silica gel column chromatography, whereby a white solid was obtained in an amount of 5.8 g in 80% yield.

FD-MS $\mathrm{C_{48}H_{40}N_2O_2}$: theoretical value 676, observed value 676

(3) Synthesis of Compound 3-79

[Chem 250]

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Compound C-23 (5 g, 7.4 mmol) and polyphosphoric acid (10 g) were loaded into a three-necked flask, and the mixture was stirred at 40° C. for 8 hours.

After the completion of the reaction, the mixture was cooled to room temperature. The sample was dissolved in water (100 mL) and $\mathrm{CH_2Cl_2}$ (100 mL) and transferred to a separating funnel, followed by extraction with $\mathrm{CH_2Cl_2}$. The resultant was dried with MgSO₄, followed by filtration and concentration. The sample was purified by silica gel chromatography. After concentration to dryness, recrystallization was carried out twice, whereby a white powder (Compound 3-79) was obtained. The obtained powder was purified by sublimation, whereby a white solid was obtained in an amount of 2.4 g in 50% yield.

FD-MS $\mathrm{C_{48}H_{36}N_2}$: theoretical value 640, observed value 640

Synthesis Example 3-12

Synthesis of Compound 3-85

[Chem 251]

566

Compound C-24 (36 g, 8.0 mmol), carbazole (2.9 g, 17.6 mmol), CuI (1.5 g, 8.0 mmol), transcyclohexane 1,2-diamine (2.7 g, 24.0 mmol), $\rm K_3PO_4$ (6.8 g, 32.0 mmol), and 1,4-dioxane (a mL) were loaded into a three-necked flask, and the mixture was refluxed under an argon atmosphere for 10 hours.

After the completion of the reaction, the resultant was cooled to room temperature. The resultant sample was transferred to a separating funnel, and 50 mL of water was charged into the funnel. Then, the mixture was extracted with CH₂Cl₂. The resultant sample was purified by silica gel column chromatography. The purified product was concentrated to dryness, and was then recrystallized twice, whereby a white powder (Compound 3-85) was obtained. The powder was purified by sublimation, whereby a white solid was obtained in an amount of 1.2 g in 25% yield.

FD-MS $C_{42}H_{24}N_2S_2$: theoretical value 620, observed value 620

An apparatus and measurement conditions adopted for field desorption mass spectrometry (FD-MS) in each of Synthesis Examples 3-1 to 3-12 are shown below.

Apparatus: HX110 (manufactured by JEOL Ltd.)

Conditions: accelerating voltage 8 kV

scan range m/z=50 to 1,500

emitter kind: carbon

emitter current: 0 mA \rightarrow 2 mA/min \rightarrow 40 mA (held for 10

minutes)

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Example 3-1

(Production of Organic EL Device)

A glass substrate provided with an ITO transparent electrode measuring 25 mm by 75 mm by 1.1 mm (manufactured by GEOMATEC Co., Ltd.) was subjected to ultrasonic cleaning in isopropyl alcohol for 5 minutes. Further, the substrate was subjected to ultraviolet (UV)-ozone cleaning for 30 minutes.

The glass substrate provided with a transparent electrode thus cleaned was mounted on a substrate holder of a vacuum deposition apparatus. First, Compound 3-A mentioned below was deposited from the vapor onto the surface of the glass substrate on the side where a transparent electrode line was formed so as to cover the transparent electrode, whereby a hole transporting layer having a thickness of 30 nm was obtained.

Compound 3-1 as a host for phosphorescence and Ir(Ph-ppy)₃ as a dopant for phosphorescence were co-deposited from the vapor onto the hole transporting layer, whereby a phosphorescent layer having a thickness of 30 nm was obtained. The concentration of Ir(Ph-ppy)₃ was 5 mass %.

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Subsequently, Compound 3-B mentioned below having a thickness of 10 nm, Compound 3-C mentioned below having a thickness of 20 nm, LiF having a thickness of 1 nm, and metal Al having a thickness of 80 nm were sequentially laminated on the phosphorescent layer, whereby a cathode was obtained. It should be noted that LiF as an electron injectable electrode was formed at a rate of 1 Å/min.

[Chem 252]

Ir(Ph-ppy)3(facial body)

(Evaluation of Organic EL Device for Light Emitting Performance)

The organic EL device thus produced was caused to emit light by being driven with a direct current. The luminance (L) of the emitted light and the current density at which the device started to emit the light were measured. Then, the current efficiency (L/J) of the device at a luminance of 1,000 cd/m² was determined. Further, the lifetime of the device at a luminance of 20,000 cd/m² was determined. Table 1 shows the results.

Examples 3-2 to 3-12

Organic EL devices were each produced in the same manner as in Example 3-1 except that a host material listed in Table 3 was used instead of Host Compound 3-1 in Example 3-1, and the devices were each evaluated in the same manner as in Example 3-1. Table 3 shows the results of the evaluation for light emitting performance.

Comparative Examples 3-1 and 3-2

Organic EL devices were each produced in the same manner as in Example 3-1 except that the following compounds (3-a) to (3-b) described in EP 0908787 A was used as a host material instead of Host Compound 3-1 in Example 3-1, and the devices were each evaluated in the same manner as in Example 3-1. Table 3 shows the results of the evaluation for light emitting performance.

Comparative Examples 3-3 to 3-5

Organic EL devices were each produced in the same manner as in Example 3-1 except that the following compounds (3-c) to (3-e) described in WO 2006-122630 was used as a host material instead of Host Compound 3-1 in Example 3-1, and the devices were each evaluated in the same manner as in Example 3-1. Table 3 shows the results of the evaluation for light emitting performance.

Comparative Example 3-6

An organic EL device was produced in the same manner as in Example 3-1 except that the following compound (3-f) described in WO 2007-063754 was used as a host material instead of Host Compound in Example 3-1, and the device was evaluated in the same manner as in Example 3-1. Table 3 shows the results of the evaluation for light emitting performance.

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-continued

-continued

	Host compound	Voltage (V) @20 mA/ cm ²	Efficiency (cd/A) @1,000 cd/m ²	Life time (hr) @20,000 cd/m ²
Example 3-1	(3-1)	6.0	62.3	200
Example 3-2	(3-17)	6.2	60.5	220
Example 3-3	(3-18)	6.3	63.8	250
Example 3-4	(3-34)	6.1	62.5	300
Example 3-5	(3-46)	6.0	61.5	250
Example 3-6	(3-49)	5.8	59.7	230
Example 3-7	(3-71)	4.7	49.8	200
Example 3-8	(3-73)	5.7	58.1	150
Example 3-9	(3-75)	4.8	50.6	180
Example 3-10	(3-76)	4.8	51.2	150
Example 3-11	(3-79)	4.8	45.3	100
Example 3-12	(3-85)	5.5	53.4	120
Comparative Example 3-1	(3-a)	4.5	23.1	50
Comparative Example 3-2	(3-b)	4.5	14.4	10
Comparative Example 3-3	(3-c)	4.8	34.1	70
Comparative Example 3-4	(3-d)	4.8	17.6	70
Comparative Example 3-5	(3-e)	6.1	40.1	80
Comparative Example 3-6	(3-f)	4.9	17.9	45

Example 4-1

(Production of Organic EL Device)

A glass substrate provided with an ITO transparent electrode measuring 25 mm by 75 mm by 1.1 mm (manufactured $^{50}~$ by GEOMATEC Co., Ltd.) was subjected to ultrasonic cleaning in isopropyl alcohol for 5 minutes. Further, the substrate was subjected to ultraviolet (UV)-ozone cleaning for 30 minutes.

The glass substrate provided with a transparent electrode 55 thus cleaned was mounted on a substrate holder of a vacuum deposition apparatus. First, Compound 4-A was deposited from the vapor onto the surface of the glass substrate on the side where a transparent electrode line was formed so as to cover the transparent electrode, whereby a hole transporting layer having a thickness of 30 nm was obtained.

(4-62) as a host for phosphorescence and Ir(Ph-ppy)3 as a dopant for phosphorescence were co-deposited from the vapor onto the hole transporting layer, whereby a phosphorescent layer having a thickness of 30 nm was obtained. The 65 concentration of Ir(Ph-ppy)3 was 10 mass %.

Subsequently, Compound (1-191) having a thickness of 10 nm, Compound 4-C having a thickness of 20 nm, LiF having

a thickness of 1 nm, and metal Al having a thickness of 80 nm were sequentially laminated on the phosphorescent layer, whereby a cathode was obtained. It should be noted that LiF as an electron injectable electrode was formed at a rate of 1 Å/min.

(Evaluation of Organic EL Device for Light Emitting Performance)

The organic EL device thus produced was caused to emit light by being driven with a direct current. The luminance (L) $\,\,$ 10 of the emitted light and the current density at which the device started to emit the light were measured. Then, the current efficiency (cd/A) of the device at a luminance of 1,000 cd/m² was determined. Further, the lifetime of the device at a luminance of 20,000 cd/m² was determined. Table 4 shows the $\,^{15}$ results.

Examples 4-2 and 4-3

Organic EL devices were each produced in the same manner as in Example 4-1 except that a host material listed in Table 4 was used instead of Host Compound (4-62) in Example 4-1, and the devices were each evaluated in the same manner as in Example 4-1. Table 4 shows the results of the 25 evaluation for light emitting performance.

Comparative Example 4-1

An organic EL device was produced in the same manner as in Example 4-1 except that: CBP was used instead of Host Compound (4-62) in Example 4-1; and BAlq was used instead of Electron Transportable Compound (1-191) in Example 4-1. Then, the device was evaluated in the same manner as in Example 4-1. Table 4 shows the results of the evaluation for light emitting performance.

Compound 4-B

55

-continued

Ir(Ph-ppy)3(facial body)

BAlq

TABLE 4

		Host compound	Electron transportable compound	Voltage (V) @20 mA/cm ²	Efficiency (cd/A) @1,000 cd/m ²	Lifetime (hr) @20,000 cd/m ²
0	Example 4-1	(4-62)	(1-191)	4.5	64.9	580
	Example 4-2	(4-1)	(1-191)	4.0	63.7	600
	Example 4-3	CBP	(1-191)	5.1	45.1	120
	Comparative Example 4-1	CBP	BAlq	6.5	45.1	30

Each of the organic EL devices of the comparative examples showed a lower current efficiency, was driven at a higher voltage, and had a shorter lifetime than those of each of the organic EL devices of the examples.

INDUSTRIAL APPLICABILITY

As described above in detail, the utilization of the polycyclic compound of the present invention represented in the general formula (1) or (2) can provide an organic EL device which shows high luminous efficiency, is free of any pixel defect, and has a long lifetime. Accordingly, the organic EL device of the present invention is extremely useful as, for example, a light source for various electronic instruments. In addition, the material can be effectively used also as a material for an organic electron device, and is extremely useful in an organic solar cell, organic semiconductor laser, a sensor using organic matter, or an organic TFT.

The invention claimed is:

1. A polycyclic compound represented by the following general formulae (7) or (8):

$$\begin{bmatrix} L_1 \\ o \\ Y_1 \end{bmatrix} = \begin{bmatrix} X_3 \\ Y_2 \\ \vdots \\ X_4 \end{bmatrix}_q$$

$$\begin{bmatrix} L_2 \\ b \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} L_2 \\ 0 \\ 0 \end{bmatrix}$$

$$X_3$$

$$X_4$$

$$\begin{bmatrix} X_4 \\ 0 \\ \vdots \\ X_4 \end{bmatrix}$$

$$\begin{bmatrix} X_1 \\ 0 \\ \vdots \\ X_4 \end{bmatrix}$$

$$\begin{bmatrix} L_1 \\ o \\ Y_1 \\ \vdots \\ L_2 \end{bmatrix}_p \qquad X_5 \qquad X_6 \qquad X_6 \qquad X_6 \qquad X_6 \qquad X_7 \qquad X_8 \qquad X_9 \qquad X_$$

where:

 X_3, X_4, X_5 , and X_6 each independently represent oxygen 45 (O), sulfur (S), or N—R₁, R₁ represents a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or $_{50}$ unsubstituted aralkyl group having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or 55 unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring, provided that when both X₃ and X₄ or both X₅ and X₆ represent N—R₁, at least one R₁ represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 60 to 24 atoms forming the aromatic ring;

o, p, and q each independently represent 0 or 1, provided that o+p is 1 or more;

 L_1 , L_2 , and L_3 each independently represent a structure $_{65}$ which is selected from the following formulae (21) to (39) and may have a substituent:

$$-N$$

$$\begin{array}{c}
N \\
N \\
N
\end{array}$$

$$\begin{array}{c}
N \\
N
\end{array}$$

(33)

(34)

-continued

-continued

Y₁, Y₂, and Y₃ each independently represent a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted aralkyl group 55 having 7 to 24 carbon atoms, a substituted or unsubstituted organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic 60 ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic ring which is bonded with a carbon atom, a number of Y_1 's is 0, 1, 2, or 3, a number of Y_2 's is 0, 1, 2, 3, or 4, and a number of Y_3 's is 0, 1, or 2.

2. The polycyclic compound according to claim 1, which is represented by any one of the following general formulae (7-1), (7-2), (8-1), and (8-2):

(7-2)

(8-1)

$$X_1$$
 X_2
 X_3
 X_4
 X_5
 X_4
 X_5
 X_5
 X_6
 X_7
 X_8
 X_8
 X_9
 X_9

3. The polycyclic compound according to claim **1**, which is represented by the following general formula (19):

- **4**. The polycyclic compound according to claim **1**, wherein a total number of substituents represented by Y_1, Y_2 , and Y_3 in the general formulae (7) and (8) is 2 or less.
- 5. The polycyclic compound according to claim 1, wherein a number of substituents represented by Y_1 and Y_2 in the general formulae (7) and (8) is 0.
- 6. The polycyclic compound according to claim 1, wherein a number of substituents represented by Y_3 in the general formulae (7) and (8) is 0.
- 7. The polycyclic compound according to claim 1, wherein o+p+q is 2 or less in the general formulae (7) and (8).
- **8**. The polycyclic compound according to claim **1**, wherein 60 o+p is 1 in the general formulae (7) and (8).
- 9. The polycyclic compound according to claim 1, wherein both X_3 and X_4 or X_5 and X_6 represent $N-R_1$ in the general formulae (7) and (8).
- 10. The polycyclic compound according to claim 1, 65 wherein both X_3 and X_4 represent N— R_1 in the general formula (7) and both R_1 's represent substituted or unsubstituted

11. The polycyclic compound according to claim 1, wherein X_3 and X_4 or X_5 and X_6 each represent N— R_1 in the general formulae (7) and (8) and N— R_1 of X_3 and N— R_1 of X_4 or N— R_1 of X_5 and N— R_1 of X_6 are different from each other.

12. The polycyclic compound according to claim 1, wherein at least one of X_3 and X_4 in the general formula (7) represents an oxygen atom, and at least one of X_5 and X_6 in the general formula (8) represents an oxygen atom.

13. The polycyclic compound according to claim 12, wherein both X_3 and X_4 or both X_5 and X_6 in the general formulae (7) and (8) represent oxygen atoms.

14. An organic electroluminescence device, comprising one or more organic thin film layers containing a light emitting layer between a cathode and an anode, wherein at least one of the organic thin film layers contains the polycyclic compound according to claim 1.

(8-2) 25 **15**. The organic electroluminescence device according to claim **14**, wherein the light emitting layer contains the polycyclic compound as a host material.

16. The organic electroluminescence device according to claim 14, wherein the light emitting layer further contains a phosphorescent material.

17. The organic electroluminescence device according to claim 14, wherein the light emitting layer contains a host material and a phosphorescent material, and the phosphorescent material comprises an orthometalated complex of an iridium (Ir), osmium (Os), or platinum (Pt) metal.

18. The organic electroluminescence device according to claim 14, further comprising an electron injecting layer between the light emitting layer and the cathode, wherein the electron injecting layer contains a nitrogen-containing ring derivative.

19. The organic electroluminescence device according to claim 14, further comprising an electron transporting layer between the light emitting layer and the cathode, wherein the electron transporting layer contains the polycylic compound.

20. The organic electroluminescence device according to claim 14, further comprising a hole transporting layer
 between the light emitting layer and the anode, wherein the hole transporting layer contains the polycyclic compound.

21. The organic electroluminescence device according to claim 14, further comprising a reducing dopant at an interfacial region between the cathode and the organic thin film layer.

22. The organic electroluminescence device according to claim 19, wherein the light emitting layer includes a material for an organic electroluminescence device which is a compound having a π -conjugated heteroacene skeleton crosslinked with a carbon atom, a nitrogen atom, an oxygen atom, or a sulfur atom as a host material.

23. The organic electroluminescence device according to claim 19, wherein the light emitting layer contains, as a host material, a material for an organic electroluminescence device represented by any one of the following general formulae (40) to (43):

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forming the aromatic ring and which is linked with a benzene ring a through a carbon-carbon bond; L₂ represents a single bond, an alkylene group having 1 to

20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with a benzene ring c through a carbon-carbon bond, provided that when both X_{15} and X_{16} or both X_{17} and X_{18} represent CR₂R₃ and both L₁ and L₂ represent substituted or unsubstituted divalent aromatic hydrocarbon groups having 6 to 24 carbon atoms forming the aromatic ring, a case where L_1 and L_2 are simultaneously linked at para position with respect to a benzene ring b is excluded;

when n represents 2, L₃ represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carbon-carbon bond, when n represents 3, L₃ represents an alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group which has 3 to 24 atoms and which is linked with the benzene ring c through a carbon-carbon bond, and when n represents 4, L₃ represents an alkanetetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carbon-carbon bond, provided that when both \boldsymbol{X}_{15} and \boldsymbol{X}_{16} or both X_{17} and X_{18} represent CR_2R_3 and both L_1 and L_3 represent substituted or unsubstituted divalent, trivalent, or tetravalent aromatic hydrocarbon groups having 6 to 24 carbon atoms forming the aromatic ring, a case where L_1 and L_3 are simultaneously linked at para position with respect to the benzene ring b is excluded;

A₁ represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic

(40)(41) 10 15 (42) 20 25 (43)35

where:

 X_{15} , X_{16} , X_{17} , and X_{18} each independently represent oxygen (O), sulfur (S), N-R₁, or CR₂R₃, R₁, R₂, and R₃ each independently represent an alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an aralkyl group having 7 to 24 carbon atoms, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group having 3 to 24 atoms forming the aromatic 55 ring, provided that when both X_{15} and X_{16} or both X_{17} and X₁₈ represent N—R₁, at least one R₁ represents a substituted or unsubstituted monovalent fused aromatic heterocyclic group having 8 to 24 atoms forming the aromatic ring;

n represents 2, 3, or 4, and the material comprises a dimer using L_3 as a linking group for n=2, a trimer using L_3 as a linking group for n=3, or a tetramer using L₃ as a linking group for n=4;

 L_1 represents a single bond, an alkylene group having 1 to 65 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms formhydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with L₁ through a carbon-carbon bond, provided that when L_1 represents an alkyl or alkylene $\,^{5}$ group having 1 to 20 carbon atoms, a case where A₁ represents a hydrogen atom is excluded;

 \mathbf{A}_2 represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and 15 which is linked with L₂ through a carbon-carbon bond, provided that when L_2 represents an alkyl or alkylene group having 1 to 20 carbon atoms, a case where A, represents a hydrogen atom is excluded;

 Y_1, Y_2 , and Y_3 each represent an alkyl group having 1 to 20 $_{\ 20}$ carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an alkoxy group having 1 to 20 carbon atoms, an aralkyl group having 7 to 24 carbon atoms, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubsti- 25 tuted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring a, b, or c through a carboncarbon bond, a number of each of Y₁ and Y₃ is 0, 1, 2, or 3, and a number of Y₂ is 0, 1, or 2, provided that when both X_{15} and X_{16} or both X_{17} and X_{18} represent oxygen (O), sulfur (S), or CR_2R_3 , both L_1 and L_2 represent $_{35}$ single bonds, and both A_1 and A_2 represent hydrogen atoms, a case where a benzene ring b has one or two Y2's, which represent a methyl group or an unsubstituted phenyl group is excluded; and

 A_1, A_2, L_1, L_2 , and L_3 are each free of any carbonyl group. A_{40} 24. The organic electroluminescence device according to claim 19, wherein the light emitting layer contains, as a host material, a material for an organic electroluminescence device represented by any one of the following general formulae (44) to (47):

$$A_1$$
 L_1 Y_2 L_2 A_2 L_3 A_4 A_4 A_5 A_5

$$A_1$$
 A_1
 A_1
 A_1
 A_1
 A_1
 A_1
 A_2
 A_2
 A_2
 A_2
 A_3
 A_4
 A_4
 A_4
 A_4
 A_5
 A_5

-continued

$$\begin{bmatrix} A_1 & L_1 & Y_2 & \\ & & b & c & \\ & & & Y_3 & \\ & & & & \end{bmatrix}_n$$

(46)

$$\begin{array}{c|c} A_1 & & \\ X_1 & & \\ X_2 & & \\ & &$$

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n represents 2, 3, or 4, and the material comprises a dimer using L₃ as a linking group for n=2, a trimer using L₃ as a linking group for n=3, or a tetramer using L₃ as a linking group for n=4;

 L_1 represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with a benzene ring a through a carbon-carbon bond;

L₂ represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with a benzene ring c through a carbon-carbon bond;

when n represents 2, L₃ represents a single bond, an alkylene group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkylene group having 3 to 20 carbon atoms forming the aromatic ring, a divalent organosilyl group having 2 to 20 carbon atoms which is bonded with a silicon atom, a substituted or unsubstituted divalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted divalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c through a carbon-carbon bond, when n represents 3, L₃ represents an alkanetriyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetriyl group having 3 to 20 carbon atoms forming the ring, a trivalent organosilyl group having 1 to 20 carbon atoms which is bonded with

a silicon atom, a substituted or unsubstituted trivalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted trivalent aromatic heterocyclic group which has 3 to 24 atoms and which is linked with the 5 benzene ring c through a carbon-carbon bond, or when n represents 4, L3 represents an alkanetetrayl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkanetetrayl group having 3 to 20 carbon atoms forming the ring, a silicon atom, a substituted or unsubstituted tetravalent aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted tetravalent aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring c $\,^{15}$ through a carbon-carbon bond;

 A_1 represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with L_1 through a carbon-carbon bond, provided that when L_1 represents an alkyl or alkylene 25 group having 1 to 20 carbon atoms, a case where A_1 represents a hydrogen atom is excluded;

A₂ represents a hydrogen atom, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms

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forming the ring, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or an aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with $\rm L_2$ through a carbon-carbon bond, provided that when $\rm L_2$ represents an alkyl or alkylene group having 1 to 20 carbon atoms, a case where $\rm A_2$ represents a hydrogen atom is excluded;

 Y_1, Y_2 , and Y_3 each represent an alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted cycloalkyl group having 3 to 20 carbon atoms forming the ring, an alkoxy group having 1 to 20 carbon atoms, an aralkyl group having 7 to 24 carbon atoms, an organosilyl group having 3 to 20 carbon atoms, a substituted or unsubstituted aromatic hydrocarbon group having 6 to 24 carbon atoms forming the aromatic ring, or a substituted or unsubstituted aromatic heterocyclic group which has 3 to 24 atoms forming the aromatic ring and which is linked with the benzene ring a, b, or c through a carboncarbon bond, a number of each of Y₁ and Y₃ is 0, 1, 2, or 3, and a number of Y_2 is 0, 1, or 2, provided that when both L_1 and L_2 represent single bonds, and both A_1 and A2 represent hydrogen atoms, a case where a benzene ring b has one or two Y2's, which represent a methyl group or an unsubstituted phenyl group is excluded; and A_1, A_2, L_1, L_2 , and L_3 are each free of any carbonyl group.

* * * * *



专利名称(译)	多环化合物和使用其的有机电致发	光器件	
公开(公告)号	<u>US8318323</u>	公开(公告)日	2012-11-27
申请号	US12/552421	申请日	2009-09-02
申请(专利权)人(译)	出光兴产股份有限公司.		
当前申请(专利权)人(译)	出光兴产股份有限公司.		
[标]发明人	KATO TOMOKI NUMATA MASAKI NISHIMURA KAZUKI IWAKUMA TOSHIHIRO HOSOKAWA CHISHIO YOSHIDA KEI		
发明人	KATO, TOMOKI NUMATA, MASAKI NISHIMURA, KAZUKI IWAKUMA, TOSHIHIRO HOSOKAWA, CHISHIO YOSHIDA, KEI		
IPC分类号	H01L51/54 C09K11/06		
CPC分类号	C07D209/86 C07D403/10 C07D487/04 C07D491/04 C07D491/048 C07D493/04 C07D495/04 C07D497 /04 C07D519/00 C09K11/06 H01L51/0072 H01L51/0073 H01L51/0074 H05B33/14 C09K2211/1007 C09K2211/1011 C09K2211/1014 C09K2211/1029 C09K2211/1044 C09K2211/1088 C09K2211/1092		
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外部链接	Espacenet USPTO		

摘要(译)

本发明提供一种化合物的多环化合物,其具有这样的结构:两个苯环彼此键合到中心苯环上以形成稠环,另一个稠环键合到其末端,以及包含一个或多个有机薄的有机电致发光器件在阴极和阳极之间包含发光层的薄膜层,其中至少一个有机薄膜层包括本发明的多环化合物。该有机电致发光器件具有高发光效率,无像素缺陷和长寿命。另外,提供了实现有机电致发光器件的多环化合物。

$$\begin{bmatrix} L_1 l_0 \\ Y_1 \end{bmatrix} A B$$

$$\begin{bmatrix} L_2 l_p \\ Y_1 \end{bmatrix} A B$$

$$\begin{bmatrix} L_1 l_0 \\ Y_1 \end{bmatrix} A B$$

$$\begin{bmatrix} L_3 a l_p \\ C_2 \end{bmatrix} \begin{bmatrix} L_3 a l_p \\ C_2 \end{bmatrix} \begin{bmatrix} L_3 a l_p \\ C_2 \end{bmatrix} \begin{bmatrix} L_3 a l_p \\ C_3 \end{bmatrix}$$

$$\begin{bmatrix} Ar_1 \\ C_4 \end{bmatrix} \begin{bmatrix} Ar_1 \\ C_4 \end{bmatrix}$$

$$\begin{bmatrix} Ar_1 \\ C_4 \end{bmatrix}$$