



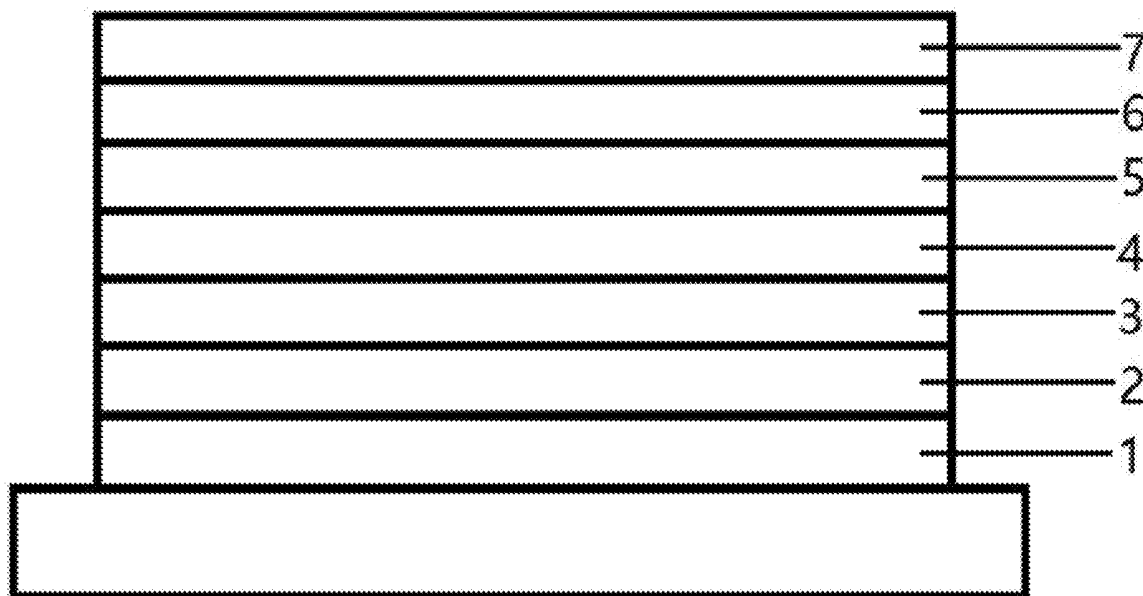
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SUN et al.(10) **Pub. No.: US 2020/0006669 A1**(43) **Pub. Date: Jan. 2, 2020**(54) **FUSED CYCLIC COMPOUND, AND
PREPARATION METHOD AND USE
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Kuan CHEN, Ningbo City (CN)**(21) Appl. No.: **16/262,228**(22) Filed: **Jan. 30, 2019**(30) **Foreign Application Priority Data**

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C07D 471/22 (2013.01); **C07D 487/22**
(2013.01); **C07D 487/16** (2013.01)(57) **ABSTRACT**

The invention relates to a fused cyclic compound having a structure of Formula compound by controlling conjugation of aromatic and heterocyclic rings. The electron transport performance balances while hole performance of the fused cyclic compound improves. The compound has high triplet energy level and glass transition temperature. The material molecule isn't prone to crystallization. The compound ensures transfer of energy to a guest material. Adjusting substituents improves electron and hole transport performances, reducing the difference between energy levels, broadening the recombination region of carriers, and preventing triplet-triplet exciton annihilation. The invention also relates to an organic light-emitting device having at least one functional layer containing the fused cyclic compound used as a host material in a light emitting layer. The energy level of the light emitting layer becomes matched with that of the carrier transport layers, reducing the driving voltage of the device while increasing luminescence efficiency of the device.



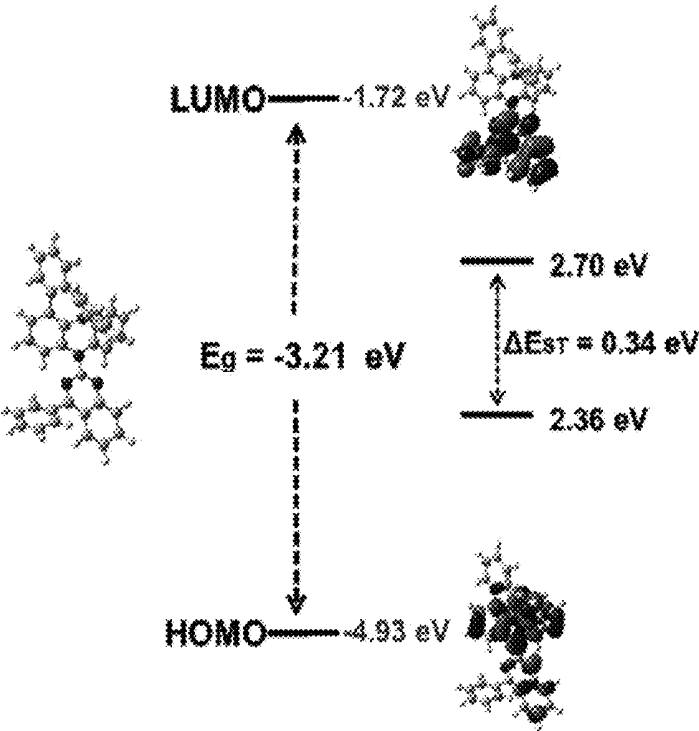


FIG. 1

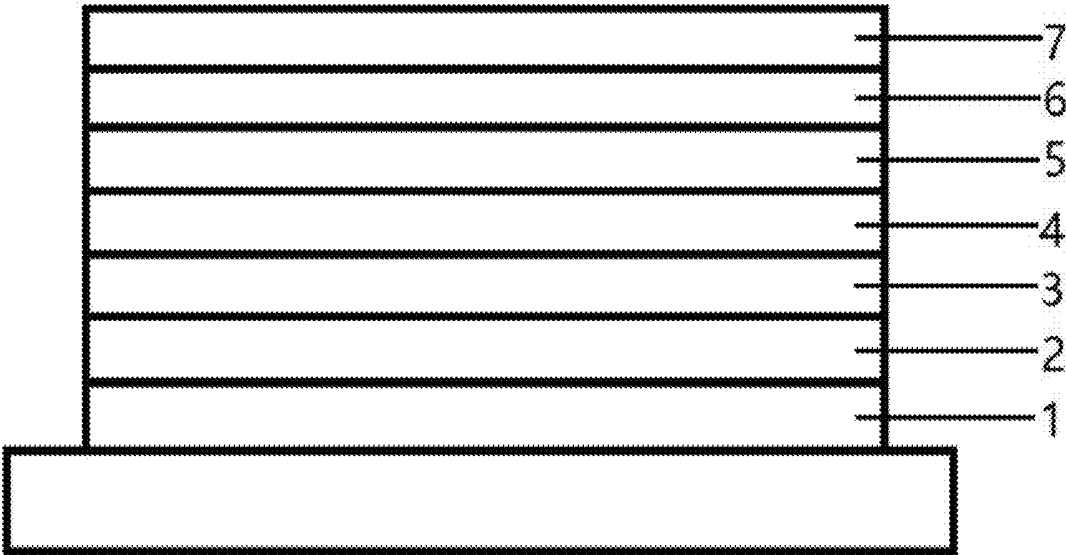


FIG. 2

FUSED CYCLIC COMPOUND, AND PREPARATION METHOD AND USE THEREOF

CROSS-REFERENCE TO RELATED APPLICATION

[0001] This application claims the priority to Chinese Patent Application No. 201810691339.9 filed on Jun. 28, 2018 with the State Intellectual Property Office of the People's Republic of China, and entitled "Fused cyclic compound and preparation method and use thereof", which is incorporated herein by reference in its entirety.

TECHNICAL FIELD

[0002] The present invention relates to the field of display technologies, and particularly to a fused cyclic compound, and a preparation method and use thereof.

RELATED ART

[0003] Pope et al. initially discovered the electroluminescence properties of single crystal anthracene in 1965. This is the first electroluminescence phenomenon of organic compounds. In 1987, a low-voltage high-brightness organic light-emitting diode (OLED) was successfully developed by Tang et al. from Kodak Company (US), using an organic small molecular semiconductor material. As a new display technology, the organic light-emitting diode (OLED) has many advantages such as self-lighting, wide viewing angle, low power consumption, rich color, fast response time, applicability over wide temperature range and flexible display, thus having broad application prospects in the field of display and illumination, and receiving more and more attention.

[0004] OLEDs often have a sandwich structure, that is, an organic light-emitting layer is sandwiched between electrodes at two sides. The light-emission mechanism is as follows. Driven by an external electric field, electrons and holes are injected into an organic electron transport layer and a hole transport layer respectively from a cathode and an anode, and recombined to form excitons in an organic light-emitting layer, and then the excitons go back to the ground state by radiation transition and emit light. In the electroluminescence process, singlet and triplet excitons are simultaneously generated. According to the statistics of electron spin, the ratio of singlet excitons to triplet excitons is inferred to be 1:3. When the singlet excitons transition back to the ground state, the material fluoresces, and when the triplet excitons transition back to the ground state, and the material phosphoresces.

[0005] Fluorescent materials are the initially used organic electroluminescent materials, which are diverse and inexpensive. However, due to the limitation by spin-forbidden transition of the electrons, only 25% of the singlet excitons can be utilized for emitting light, so the internal quantum efficiency is low, which limits the efficiency of the device. For phosphorescent materials, by means of the spin coupling of heavy atoms, the energy of singlet excitons is allowed to be transferred to triplet excitons by intersystem crossing (ISC), and then triplet excitons phosphoresce. Accordingly, an internal quantum efficiency of 100% is theoretically achievable. However, concentration quenching and triplet-triplet annihilation are common in phosphorescent devices, which affects the luminescence efficiency of the devices.

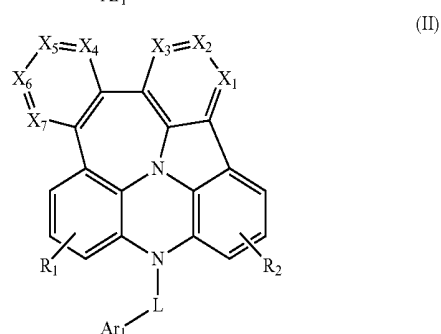
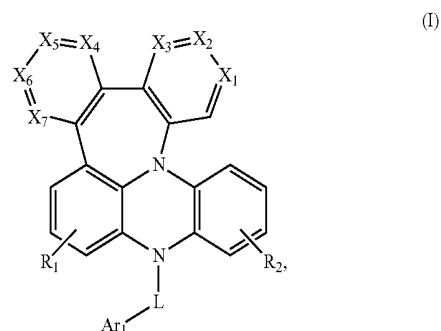
[0006] The OLED devices fabricated by the doping method are advantageous in the luminescence efficiency of the devices. Therefore, the material of the light-emitting layer is often formed by doping a guest material into a host material, where the host material is an important factor affecting the luminescence efficiency and performance of the OLED devices. 4,4'-Bis(9H-carbazol-9-yl)biphenyl (CBP) is a widely used host material with good hole transport performance. However, when CBP is used as a host material, the molecular packing state and the film morphology are prone to change and the molecules tend to recrystallize under working conditions due to the low glass transition temperature of CBP, causing decreased performance and luminescence efficiency of the OLED device during use. Moreover, CBP is a hole-type host material, the transport of electrons and holes is unbalanced, the efficiency of recombination into excitons is low, the light-emitting region is not desirable, the roll-off phenomenon of the device is serious during operation, and the triplet energy of CBP is lower than that of the blue dopant material, resulting in a low efficiency of energy transfer from the host material to the guest material, thus reducing the efficiency of the devices.

SUMMARY

[0007] Therefore, the technical problems to be solved by the present invention are to overcome the disadvantages in the prior art of low triplet energy level and tendency to crystallization of the host material in the light-emitting layer, as well as unbalanced charge transport of the host material, undesirable light-emitting region, and inability of efficiently transporting the energy of the host material to the guest material, resulting in low luminescence efficiency and performance of the devices.

[0008] To this end, the present invention provides the following technical solutions.

[0009] In a first aspect, the present invention provides a fused cyclic compound, having a structure of Formula (I) or (II):



[0010] where X_1 is selected from N or C— R_{1a} , X_2 is selected from N or C— R_{2a} , X_3 is selected from N or C— R_{3a} , X_4 is selected from N or C— R_{4a} , X_5 is selected from N or C— R_{5a} , X_6 is selected from N or C— R_{6a} , and X_7 is selected from N or C— R_{7a} , in which

[0011] R_{1a} – R_{7a} are each independently selected from hydrogen, halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, silyl, aryl or heteroaryl;

[0012] R_1 and R_2 are each independently selected from hydrogen, halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, silyl, aryl or heteroaryl;

[0013] L is a single bond, a C_1 – C_{10} substituted or unsubstituted aliphatic hydrocarbon group, a C_6 – C_{60} substituted or unsubstituted aryl group, or a C_3 – C_{30} substituted or unsubstituted heteroaryl group; and

[0014] Ar_1 is selected from hydrogen, halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, silyl, aryl or heteroaryl, in which

[0015] the heteroaryl has at least one heteroatom independently selected from nitrogen, sulfur, oxygen, phosphorous, boron or silicon.

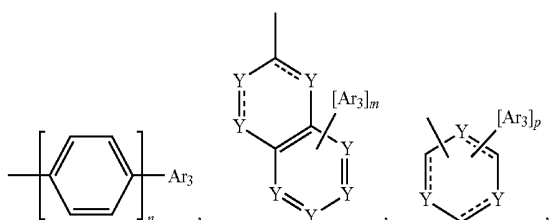
[0016] Preferably, in the fused cyclic compound,

[0017] R_1 and R_2 are each independently selected from hydrogen, halo, cyano, a C_1 – C_{30} substituted or unsubstituted alkyl group, a C_2 – C_{30} substituted or unsubstituted alkenyl group, a C_2 – C_{30} substituted or unsubstituted alkynyl group, a C_3 – C_{30} substituted or unsubstituted cycloalkyl group, a C_1 – C_{30} substituted or unsubstituted alkoxy group, a C_1 – C_{30} substituted or unsubstituted silyl group, a C_6 – C_{60} substituted or unsubstituted aryl group, or a C_3 – C_{30} substituted or unsubstituted heteroaryl group;

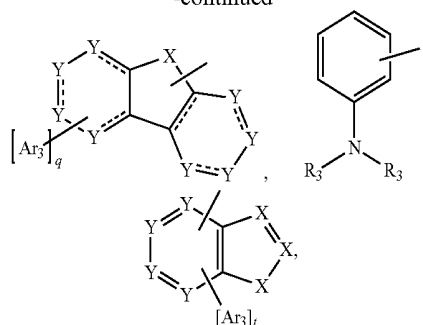
[0018] Ar_1 is selected from hydrogen, halo, cyano, a C_1 – C_{30} substituted or unsubstituted alkyl group, a C_2 – C_{30} substituted or unsubstituted alkenyl group, a C_2 – C_{30} substituted or unsubstituted alkynyl group, a C_3 – C_{30} substituted or unsubstituted cycloalkyl group, a C_1 – C_{30} substituted or unsubstituted alkoxy group, a C_1 – C_{30} substituted or unsubstituted silyl group, a C_6 – C_{60} substituted or unsubstituted aryl group, or a C_3 – C_{30} substituted or unsubstituted heteroaryl group; and

[0019] R_{1a} – R_{7a} are each independently selected from hydrogen, halo, cyano, a C_1 – C_{30} substituted or unsubstituted alkyl group, a C_2 – C_{30} substituted or unsubstituted alkenyl group, a C_2 – C_{30} substituted or unsubstituted alkynyl group, a C_3 – C_{30} substituted or unsubstituted cycloalkyl group, a C_1 – C_{30} substituted or unsubstituted alkoxy group, a C_1 – C_{30} substituted or unsubstituted silyl group, a C_6 – C_{60} substituted or unsubstituted aryl group, or a C_3 – C_{30} substituted or unsubstituted heteroaryl group.

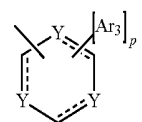
[0020] Preferably, in the fused cyclic compound, Ar_1 is selected from any of the following groups, and R_1 , R_2 , R_{1a} , R_{2a} , R_{3a} , R_{4a} , R_{5a} , R_{6a} , and R_{7a} are each independently selected from hydrogen or any of the following groups:



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[0021] where X is nitrogen, oxygen or sulfur, Y is each independently nitrogen or carbon; and in the



at least one Y is nitrogen; and

[0022] n is an integer of 0-5, m is an integer of 0-7, p is an integer of 0-6, q is an integer of 0-8, and t is an integer of 0-7; and --- is a single or double bond;

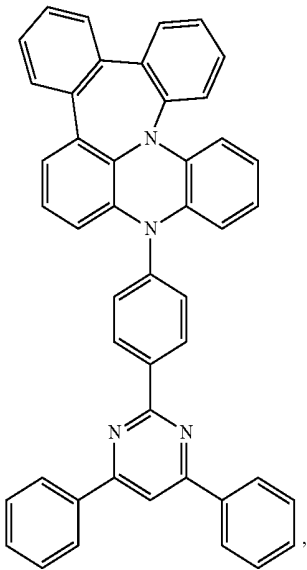
[0023] R_3 is each independently selected from a substituted or unsubstituted phenyl group or hydrogen; and

[0024] Ar_3 is each independently selected from hydrogen, phenyl, coronenyl, pentalenyl, indenyl, naphthyl, azulenyl, fluorenyl, heptalenyl, octalenyl, benzodiindenyl, acenaphth-ylenyl, phenalenyl, phenanthrenyl, anthracenyl, triindenyl, fluoranthrenyl, benzopyrenyl, benzoperilenyl, benzofluoranthrenyl, acephenanthrenyl, aceanthrylenyl, 9,10-benzophenanthrenyl, pyrenyl, 1,2-benzophenanthrenyl, butylphenyl, naphthacenyl, pleiadenyl, picenyl, perylenyl, pentaphenyl, pentacenyl, tetraphenylene, cholanthrenyl, helicenyl, hexaphenyl, rubicenyl, coronenyl, trinaphthyl-enyl, heptaphenyl, pyranthrenyl, ovalenyl, corannulenyl, anthanthrenyl, truxenyl, pyranyl, benzopyranyl, furyl, benzofuryl, isobenzofuryl, oxanthracenyl, oxazolinenyl, dibenzofuryl, peri-xanthenoxanthrenyl, thienyl, thioxanthrenyl, thianthrenyl, phenoxathiinyl, thionaphthenyl, isothionaphthenyl, thiophanthrenyl, dibenzothieryl, benzothieryl, pyrrolyl, pyrazolyl, tellurazolyl, selenazolyl, thiazolyl, isothiazolyl, oxazolyl, oxadiazolyl, furazanyl, pyridinyl, pyrazinyl, pyrimidinyl, pyridazinyl, triazinyl, indolizinenyl, indolyl, isoindolyl, indazolyl, purinyl, quinolizinenyl, isoquinolyl, carbazolyl, fluorencarbazolyl, indolocarbazolyl, imidazolyl, naphthyridinyl, phthalazinyl, quinazolinyl, benzodiazepinyl, quinoxalinyl, cinnolinyl, quinolyl, pteridinyl, phenanthridinyl, acridinyl, perimidinyl, phenanthrolinyl, phenazinyl, carbolinyl, phenotellurazinyl, phenoselenazinyl, phenothiazinyl, phenoxazinyl, triphenodithiazinyl, azadibenzofuryl, triphenodioxazinyl, anthrazinyl, benzothiazolyl, benzoimidazolyl, benzoxazolyl, benzisoxazolyl or benzoisothiazolyl.

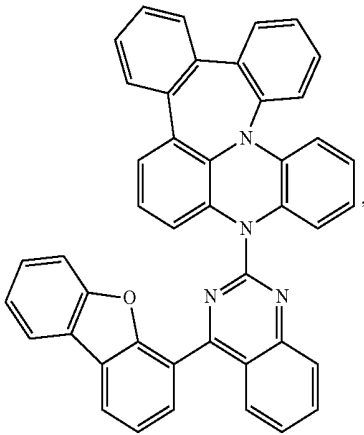
[0025] Preferably, the fused cyclic compound having a molecular structure shown below:

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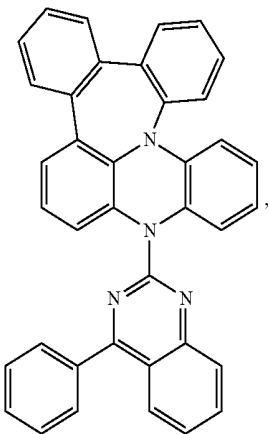
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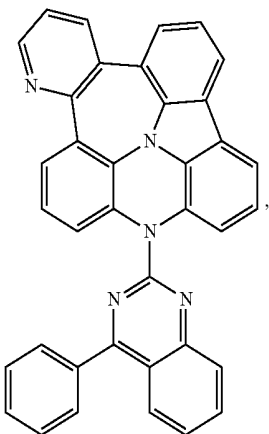
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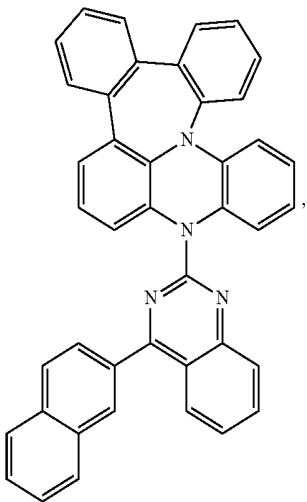
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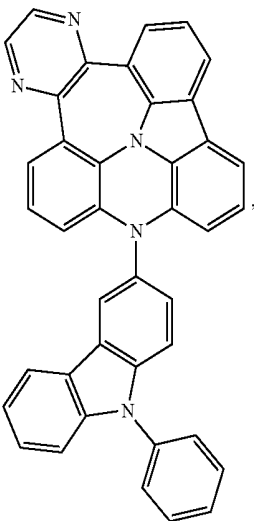
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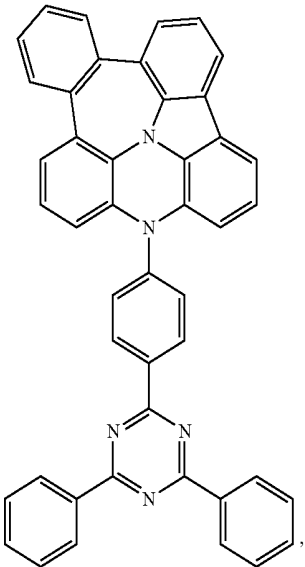
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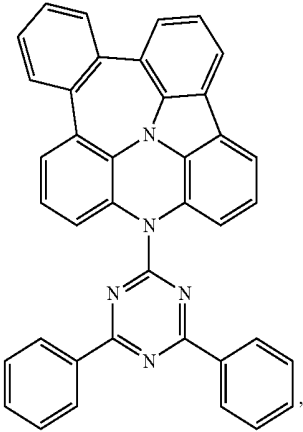
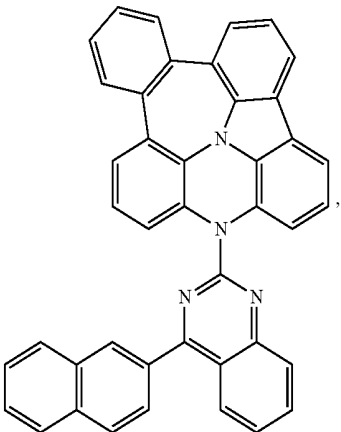
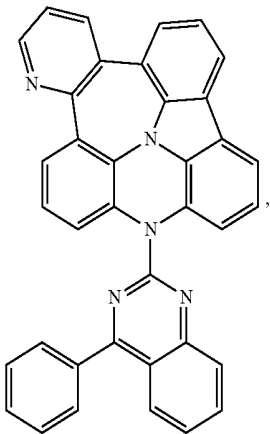
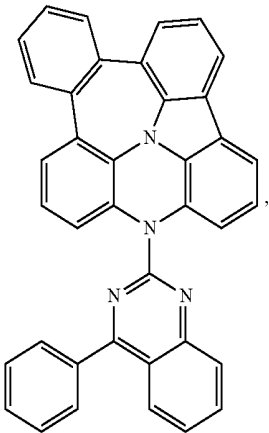
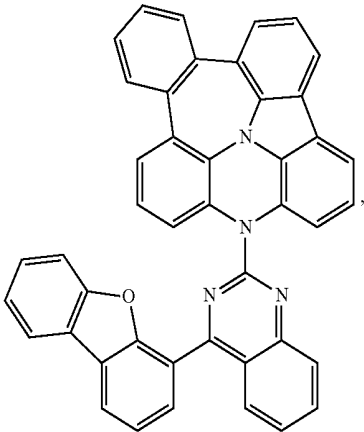
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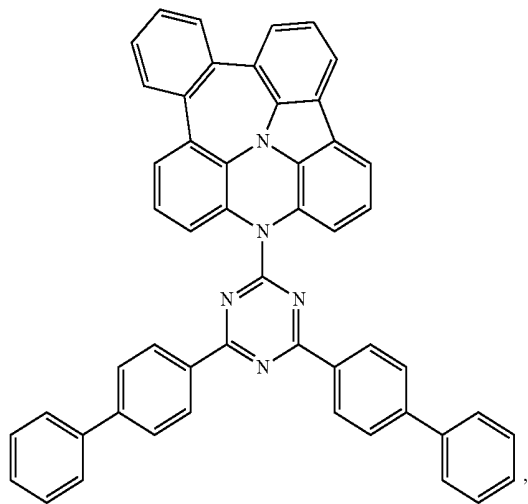


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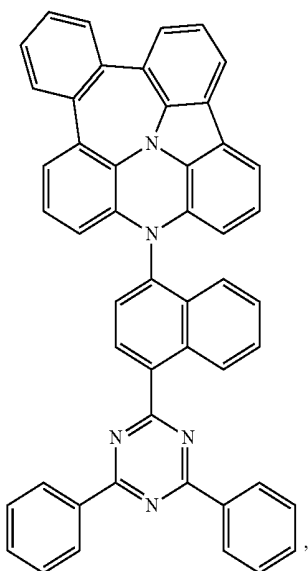


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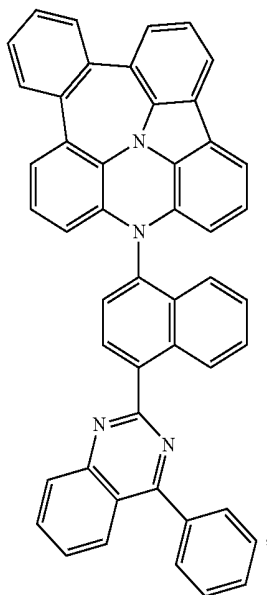
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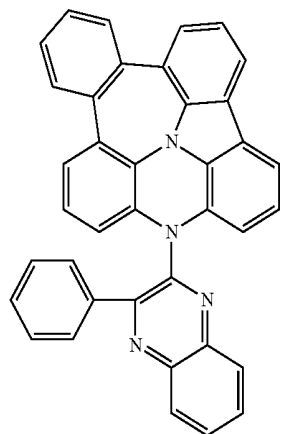


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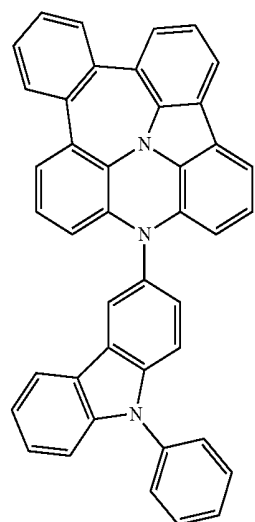


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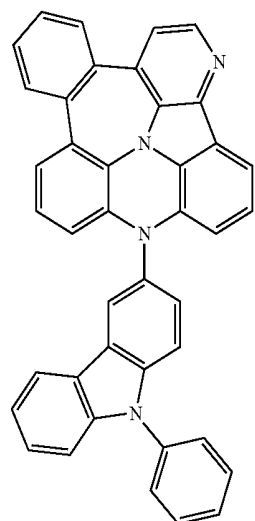
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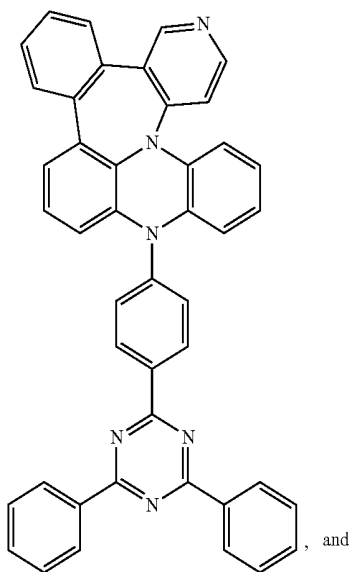
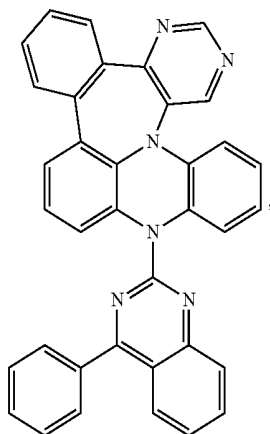
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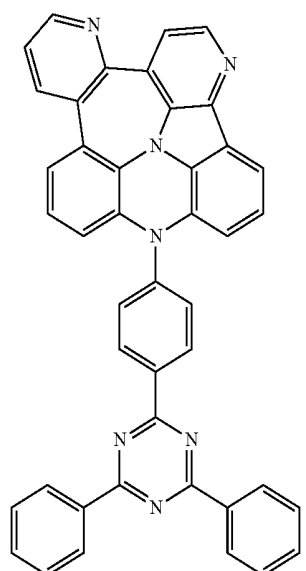
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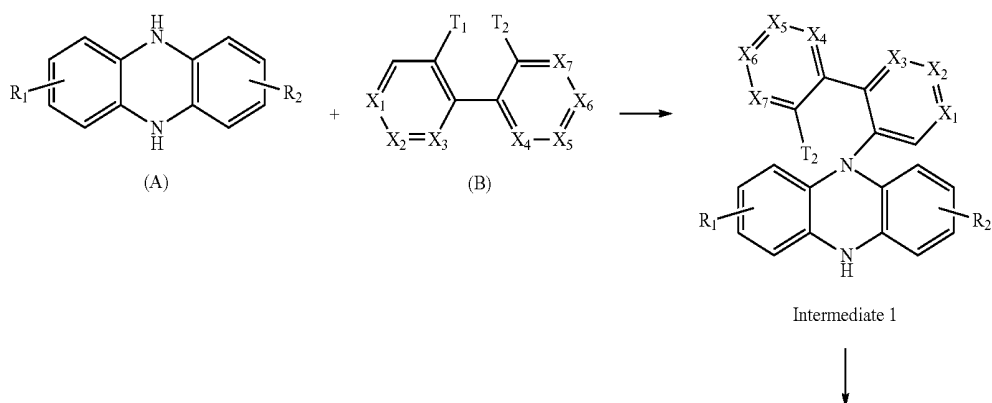


[0026] In a second aspect, the present invention provides a method for preparing the fused cyclic compound.

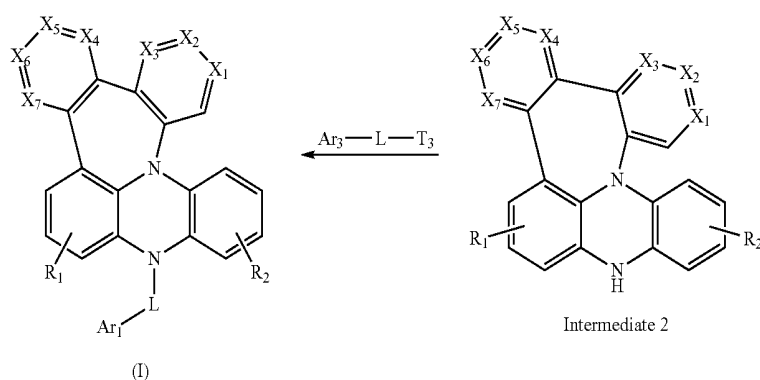
[0027] The compound of Formula (I) is synthesized through the following steps:

[0028] subjecting a compound of Formula (A) and a compound of Formula (B) as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 1; cyclizing the intermediate 1, to obtain an intermediate 2; and subjecting the intermediate 2 and a compound T_3 -L-Ar₁ to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (I).

[0029] The synthesis route for the compound of Formula (I) is shown below:



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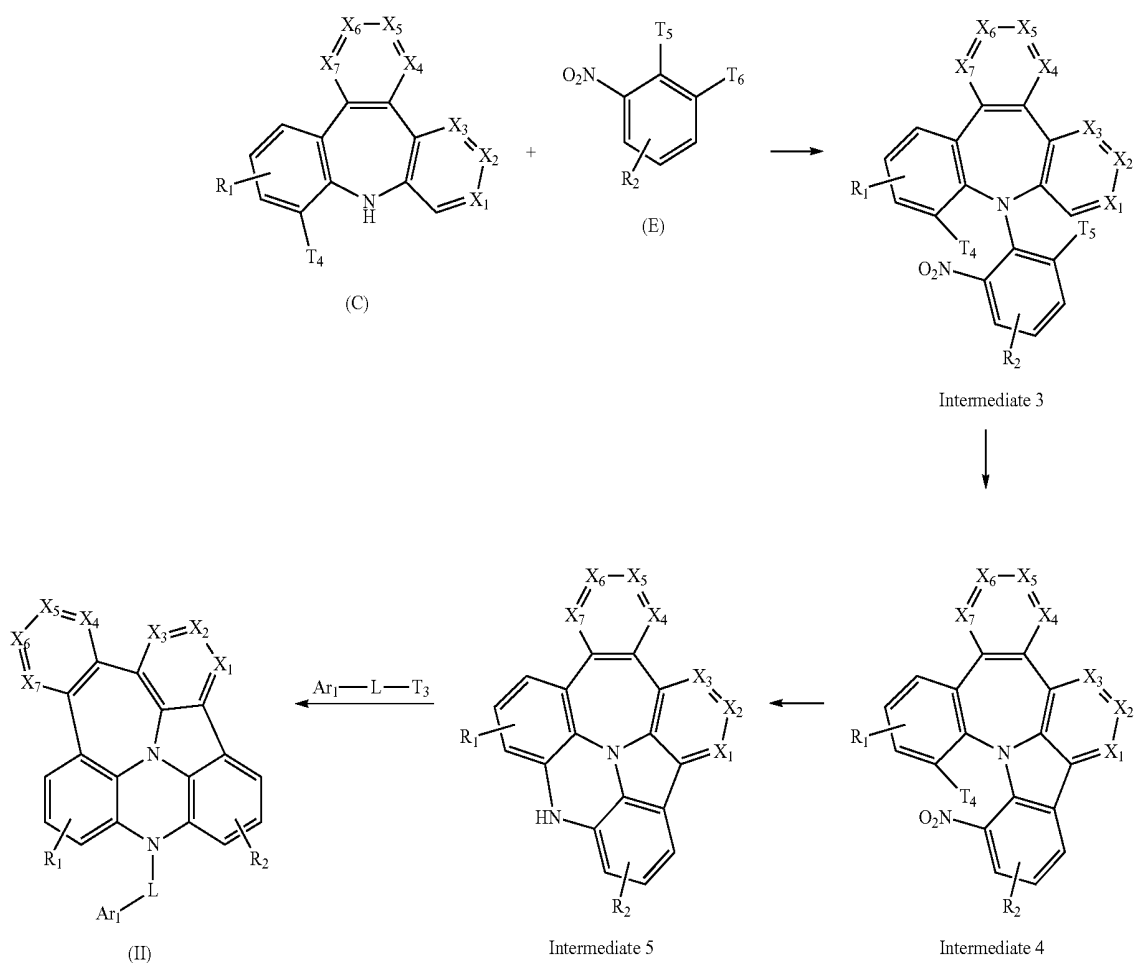


[0030] The compound of Formula (II) is synthesized through the following steps:

[0031] subjecting a compound of Formula (C) and a compound of Formula (E) as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 3; cyclizing the intermediate 3, to obtain an intermediate 4; reducing the nitro group of the intermediate 4 and

then subjecting the intermediate 4 to a coupling reaction, to obtain an intermediate 5; and subjecting the intermediate 5 and a compound T_3-L-Ar_1 to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (II).

[0032] The synthesis route for the compound of Formula (II) is shown below:



[0033] where T_1 - T_6 are each independently selected from hydrogen, fluoro, chloro, bromo or iodo.

[0034] In a third aspect, the present invention provides a method for preparing the fused cyclic compound.

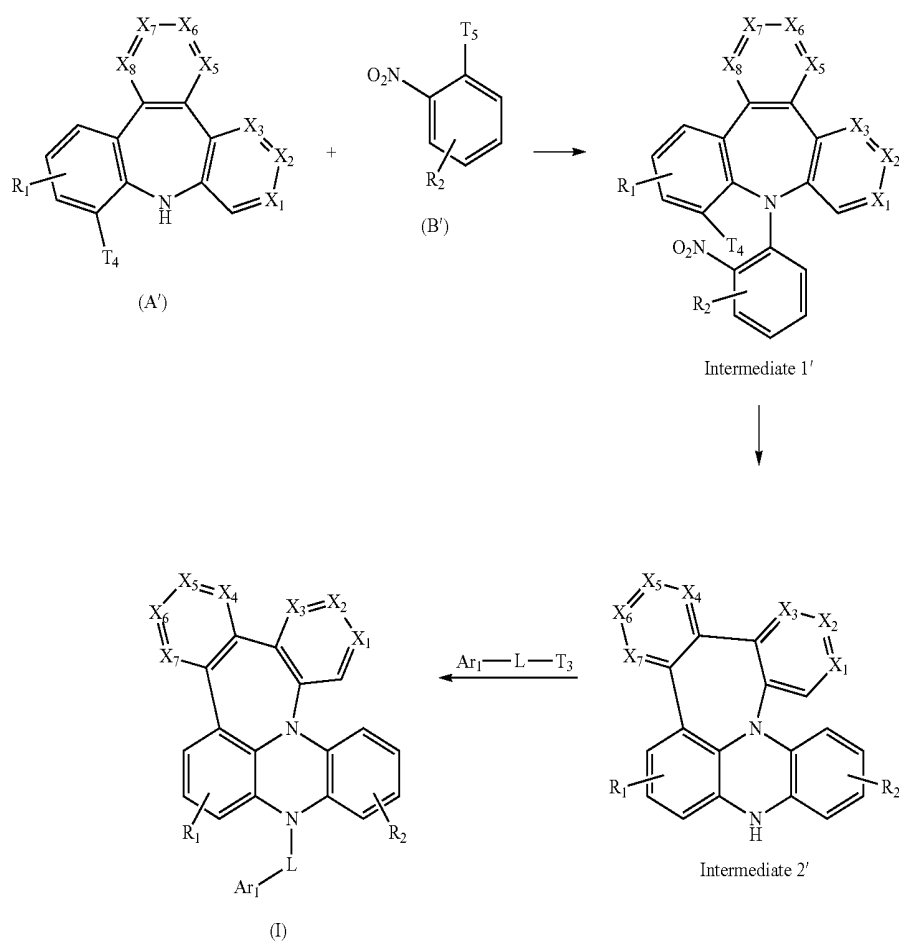
[0035] The compound of Formula (I) is synthesized through the following steps:

[0036] subjecting a compound of Formula (A') and a compound of Formula (B') as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 1'; cyclizing the intermediate 1', to obtain an intermediate 2'; and subjecting the intermediate 2' to a compound T_3 -L- Ar_1 to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (I).

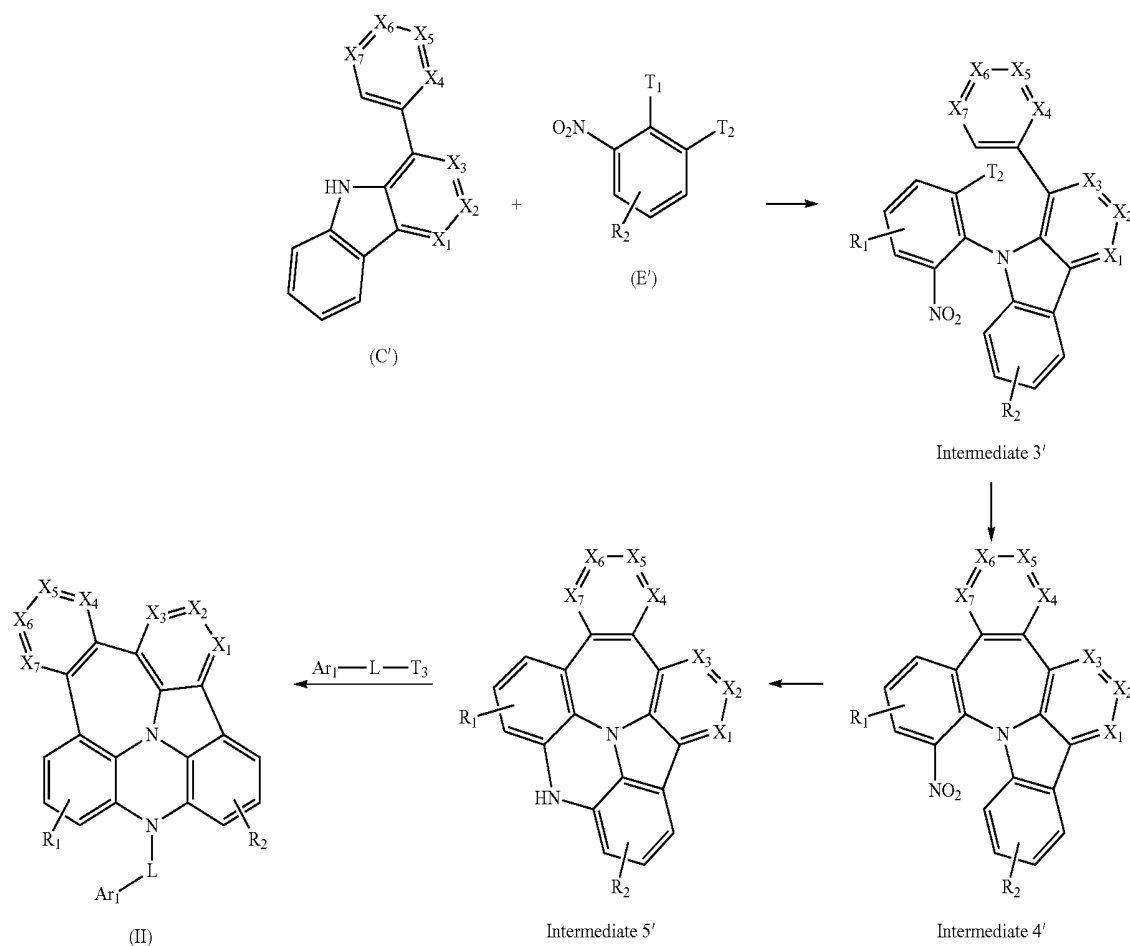
[0037] The synthesis route for the compound of Formula (I) is shown below:

[0038] The compound of Formula (II) is synthesized through the following steps:

[0039] subjecting a compound of Formula (C') and a compound of Formula (E') as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 3'; cyclizing the intermediate 3', to obtain an intermediate 4'; reducing the nitro group of the intermediate 4' and then subjecting the intermediate 4' to a coupling reaction, to obtain an intermediate 5'; and subjecting the intermediate 5' and a compound T_3 -L- Ar_1 to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (II).



[0040] The synthesis route for the compound of Formula (II) is shown below:



[0041] where T_1 - T_5 are each independently selected from hydrogen, fluoro, chloro, bromo or iodo.

[0042] In a fourth aspect, the present invention provides use of the fused cyclic compound as an organic electroluminescent material.

[0043] In a fifth aspect, the present invention provides an organic light-emitting device, having at least one functional layer containing the fused cyclic compound.

[0044] Preferably, in the organic light-emitting device, the functional layer is a light-emitting layer.

[0045] Further preferably, the material of the light-emitting layer in the organic light-emitting device comprises a host material and a guest luminescent dye, where the host material is the fused cyclic compound.

[0046] The technical solution of the invention has the following advantages.

[0047] 1. The fused cyclic compound provided in present invention has a structure of Formula (I) or (II). The fused cyclic compound has increased effective conjugation of the mother nuclear structure by designing the fusion mode of the aromatic ring and the heterocyclic ring in the mother nuclear structure, and facilitates the balancing of the electron transport performance of material molecules while improving the hole performance of the fused cyclic compound. By controlling the degree of conjugation of the molecules, the

HOMO level of the fused cyclic compound is increased, and the difference between the singlet energy level and the triplet energy level of the molecule of material is reduced. When the material is used as a host material in the light-emitting layer, the HOMO level of the light-emitting layer can be made more matched with that of the hole injection layer, thus facilitating the injection of holes.

[0048] By configuring X_1 - X_7 , the fused cyclic compound is allowed to have both electron transport performance and hole transport performance. When the fused cyclic compound is used as a host material in the light-emitting layer, the ratio of electrons and holes in the light-emitting layer can be balanced, the carrier recombination probability is improved, and the carrier recombination region is widened, thereby improving the luminescence efficiency.

[0049] On the other hand, the fused cyclic compound of Formula (I) or Formula (II) has a high triplet energy level (T_1) and a high glass transition temperature, and can promote the effective energy transfer from the host material to the guest material, reduce the returning of the energy and improve the luminescence efficiency of OLED devices, due to the high triplet energy level when used as a host material in the light emitting layer. The fused cyclic compound has a high glass transition temperature, high thermal stability and morphological stability, and excellent film forming perfor-

mance, and is not prone to crystallization when used as a host material in the light emitting layer, thus facilitating the improvement of the performance and luminescence efficiency of the OLED device.

[0050] 2. In the fused cyclic compound provided in the invention, by adjusting the substituents R_1 , R_2 , R_{1a} - R_{7a} , and Ar_1 , an electron withdrawing group (pyridine, pyrimidine, triazine, pyrazine, oxadiazole, thiadiazole, quinazoline, imidazole, quinoxaline, quinoline, and the like), or an electron donating group (diphenylamine, triphenylamine, fluorene, and the like) can be introduced on the substituents, where the HOMO level is distributed on the electron donating group, and the LUMO level is distributed on the electron withdrawing group, such that the hole transport performance and the electron transport performance of the material molecules are further improved, and the balance of charge transfer is improved. When the material is used as a host material in the light emitting layer, the recombination region of holes and electrons is further enlarged, and the exciton concentration per unit volume is diluted to prevent concentration quenching or triplet-triplet exciton annihilation of triplet excitons due to high concentration. By configuring the electron donating group and the electron withdrawing group, the HOMO level of the fused cyclic compound is improved, and the LUMO level is lowered. When the material is used as a host material in the light emitting layer, the adjacent hole- and electron-type carrier functional layers are allowed to become more matched.

[0051] In the fused cyclic compound as shown in FIG. 1 (the compound shown in FIG. 1 is the fused cyclic compound D-2), the HOMO level and LUMO level are distributed on different electron donating group and electron withdrawing group, such that the HOMO level is effectively segregated from the LUMO level. This reduces the difference ΔE_{st} (≤ 0.3 eV) between the singlet and triplet energy levels of the material molecule, thus facilitating the reverse intersystem crossing of the triplet excitons to singlet excitons, promoting the Föster energy transfer from the host material to the guest material, and reducing losses generated during energy transfer.

[0052] By configuring the electron-donating group, the electron withdrawing group and their spatial positions, a twisted rigid molecular configuration is attained, and the degree of intermolecular conjugation is adjusted to further increase the triplet energy level of the material molecule, so a small ΔE_{st} is achieved. Moreover, by configuring L and Ar_1 , and adjusting the electron-donating group, the electron withdrawing group, and the spacing therebetween, the LUMO level or the HOMO level is allowed to distribute more evenly, thus further optimizing the HOMO and LUMO levels.

[0053] 3. The preparation method of the fused cyclic compound provided in the present invention has the advantages of readily available starting materials, mild reaction conditions, and simple operation steps, so a simple and easy-to-implement preparation method is provided for the mass production of the above fused cyclic compound.

[0054] 4. The organic light-emitting diode (OLED) device provided in the present invention has at least one functional layer containing the fused cyclic compound, where the functional layer is a light emitting layer.

[0055] The fused cyclic compound makes the electron and hole transport performances balanced, and increases the recombination probability of electrons and holes in the light

emitting layer. Moreover, the fused cyclic compound has a high triplet energy level, which facilitates the energy transfer of the host material to the guest material and prevents the returning of energy. The high glass transition temperature of the fused cyclic compound prevents crystallization of the material molecules of the light emitting layer and improves the performance of the OLED device during use.

[0056] By adjusting the substituents, the electron and hole transport performances of the fused cyclic compound are further improved, and the transport of charges and holes in the light emitting layer becomes more balanced, thereby expanding the area where holes and electrons are recombined into excitons in the light emitting layer, reducing the exciton concentration, preventing the triplet-triplet annihilation of the device, and improving the efficiency of the device; and also the carrier recombination region is allowed to stay far away from the interface of the light emitting layer to the hole or electron transport layer, thus improving the color purity of the OLED device, avoiding the returning of excitons to the transport layer, and further improving the efficiency of the device.

[0057] In the fused cyclic compound, an electron donating group and an electron withdrawing group are utilized to adjust the HOMO level and the LUMO level of the material molecules, so that the overlap between the HOMO level and the LUMO level is reduced and the fused ring has a small ΔE_{st} , which promotes the reverse intersystem crossing (RISC) of triplet excitons to singlet excitons, thereby suppressing the Dexter energy transfer (DET) from the host material to the luminescent dye, promoting the Föster energy transfer, and reducing the energy loss during the Dexter energy transfer (DET). In this way, the efficiency roll-off of the organic light-emitting device is effectively reduced, and the external quantum efficiency of the device is improved.

BRIEF DESCRIPTION OF THE DRAWINGS

[0058] In order to more clearly explain the technical solutions in the specific embodiments of the present invention or in the prior art, the drawings used in the description of the specific embodiments or the prior art will be briefly described below. Obviously, the drawings depicted below are merely some embodiments of the present invention, and those skilled in the art can obtain other drawings based on these drawings without any creative efforts.

[0059] FIG. 1 is a view showing the theoretical calculation results of HOMO level, LOMO level and ΔE_{st} of the fused cyclic compound D-2 prepared in Example 1 of the present invention; and

[0060] FIG. 2 is a schematic structural view of an organic light-emitting device according to Examples 7 to 12 and Comparative Example 1 of the present invention.

LIST OF REFERENCE NUMERALS

[0061] 1—anode, 2—hole injection layer, 3—hole transport layer, 4—light emitting layer, 5—electron transport layer, 6—electron injection layer, 7—cathode.

DETAILED DESCRIPTION

[0062] The technical solutions of the present invention will be described clearly and fully with reference to the accompanying drawings. Apparently, the embodiments described are some preferred embodiments, rather than all of

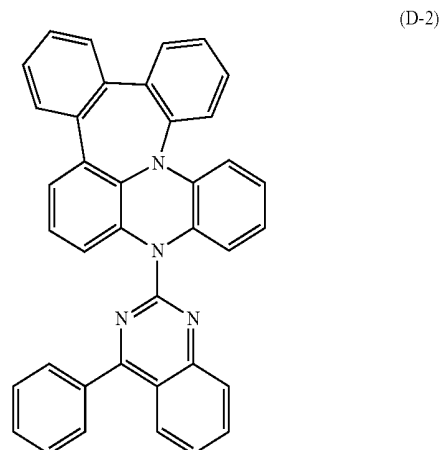
the embodiments of the present invention. All other embodiments obtained by a person of ordinary skill in the art without creative efforts based on the embodiments of the present invention shall fall within the protection scope of the present invention.

[0063] It is to be understood that in the description of the present invention, the terms “first” and “second” are used herein for purposes of description, and are not intended to indicate or imply relative importance.

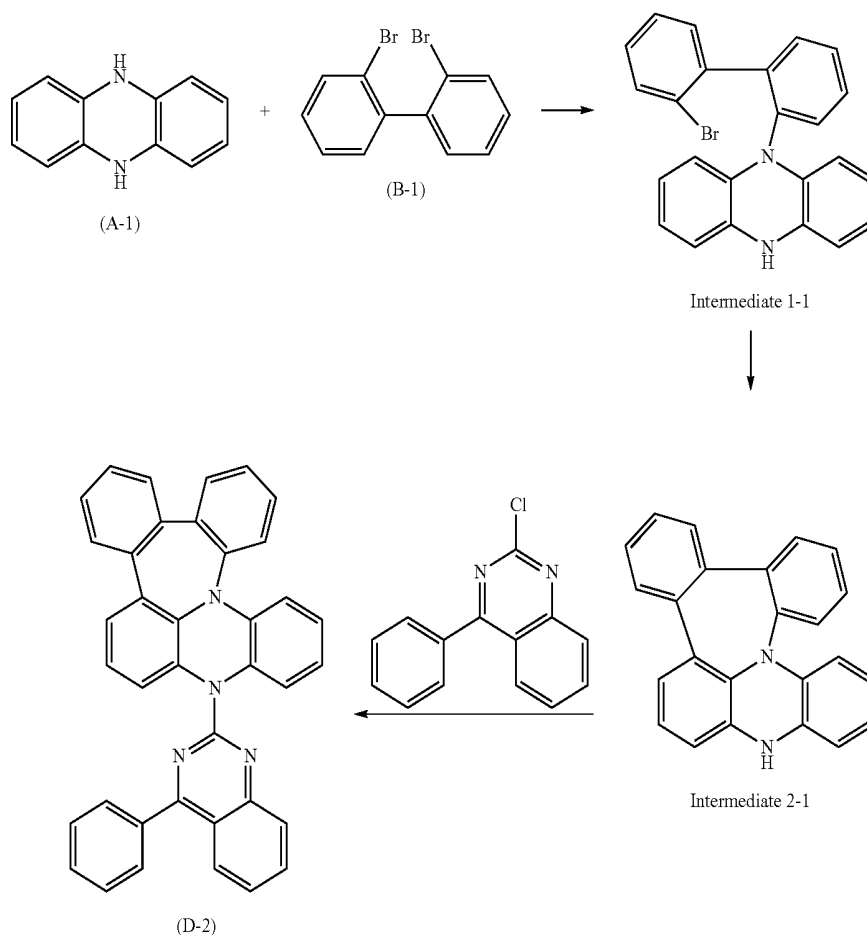
[0064] The present invention can be embodied in many different forms and is not limited to the embodiments described herein. Conversely, these embodiments are provided for the purpose of making the disclosure of the present invention more thorough and comprehensive and conveying the concept of the present invention fully to those skilled in the art, and the scope of the present invention is defined merely by the claims. In the figures, for the sake of clarity, the dimensions and relative dimensions of the layers and regions will be exaggerated. It should be understood that when an element, for example, a layer, is referred to as being “formed” or “disposed” “on” another element, the element may be directly disposed on the other element or an intervening element may be present. Conversely, when an element is referred to as being “directly formed on” or “directly disposed on” another element, no intervening element is present.

Example 1

[0065] This example provides a fused cyclic compound having a structure of Formula D-2 below:



[0066] The synthesis route for the fused cyclic compound of Formula D-2 is shown below:



[0067] The method for preparing the fused cyclic compound of Formula D-2 comprises specifically the following steps.

(1) Synthesis of Intermediate 1-1

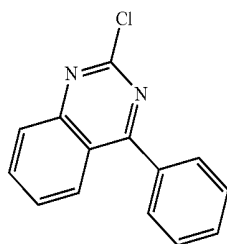
[0068] Under nitrogen atmosphere, a compound of Formula (A-1) (9.1 g, 50 mmol), 2,2'-dibromobiphenyl (a compound of Formula (B-1)) (7.8 g, 25 mmol), 1,4-dioxane (200 mL), cuprous iodide (48 mg, 0.25 mmol), sodium-*t*-butoxide (3.5 g, 36 mmol), and *cis*-1,2-cyclohexanediamine (0.3 mL) were added to a 500 mL three-neck flask, and reacted at 100° C. for 12 hrs. The reaction solution was extracted with chloroform (3×), and the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 1-1 as a solid (6.2 g, yield 60%).

(2) Synthesis of Intermediate 2-1

[0069] Under nitrogen atmosphere, the intermediate 1-1 (4.13 g, 10 mmol), potassium *tert*-butoxide (2.2 g, 23 mmol), and dimethyl sulfoxide (500 mL) were weighed to a 1 L three-neck flask, and reacted for 2 hrs under irradiation. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 2-1 as a solid (1.7 g, yield 50%).

(3) Synthesis of Fused Cyclic Compound D-2

[0070] Under nitrogen atmosphere, the intermediate 2-1 (1.7 g, 5 mmol), the compound

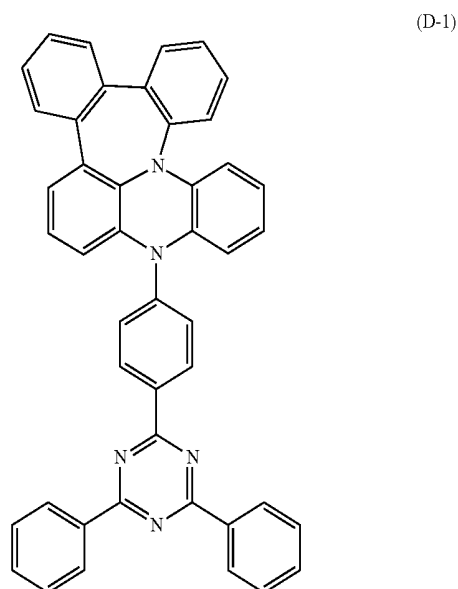


(1.6 g, 6 mmol), cesium carbonate (1.7 g, 5 mmol), 4-dimethylamino pyridine (0.3 g, 2.5 mmol), and dimethyl sulfoxide (20 mL) were added, reacted at 100° C. for 3 hrs, and then cooled to room temperature. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the fused cyclic compound D-2 as a solid (2.3 g, yield 85%).

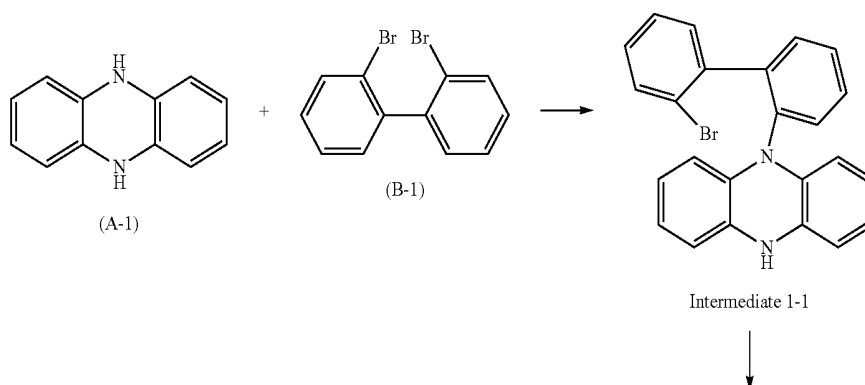
[0071] Element analysis: (C₃₈H₂₄N₄) calculated: C, 85.05; H, 4.51; N, 10.44. found: C, 85.01; H, 4.53; N, 10.45, HRMS (ESI) *m/z* (*M*⁺): calculated: 536.20. found: 536.23.

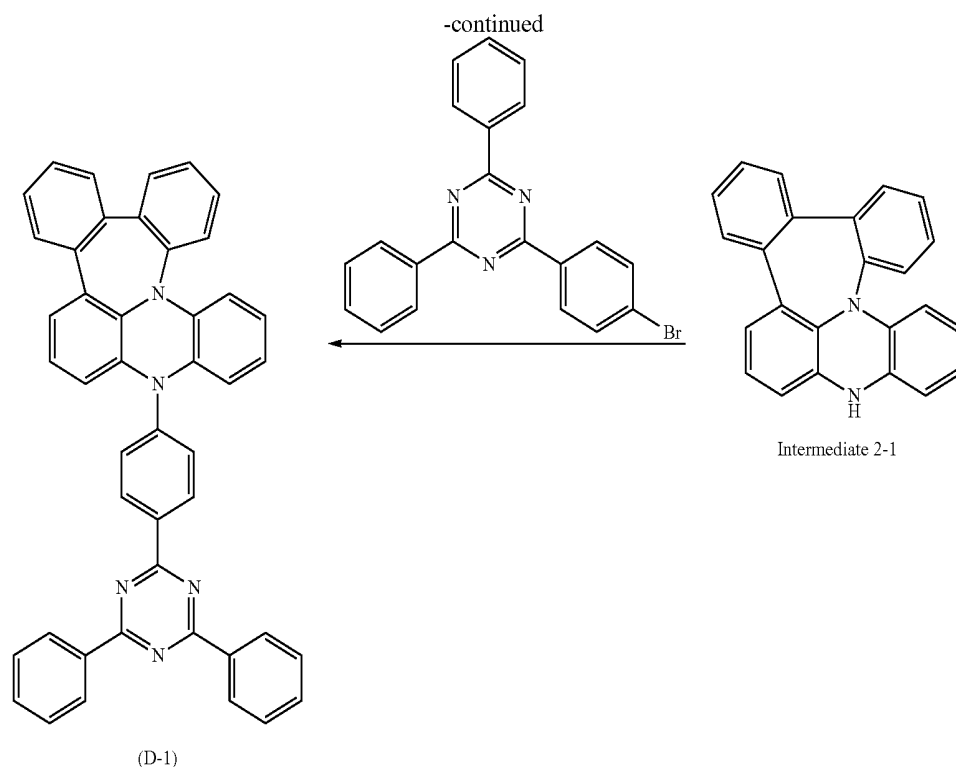
Example 2

[0072] This example provides a fused cyclic compound having a structure of Formula D-1 below:



[0073] The synthesis route for the fused cyclic compound of Formula D-1 is shown below:





[0074] The method for preparing the fused cyclic compound of Formula D-1 comprises specifically the following steps.

[0075] (1) The intermediate 2-1 was synthesized following the method as described in Example 1.

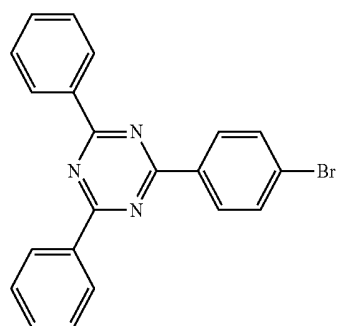
[0076] (2) Synthesis of Fused Cyclic Compound D-1

[0077] Under nitrogen atmosphere, the compound 1-2 (1.7 g, 5 mmol), palladium diacetate (0.03 g, 0.15 mmol), tri-*tert*-butylphosphine (0.1 g, 0.55 mmol), the compound

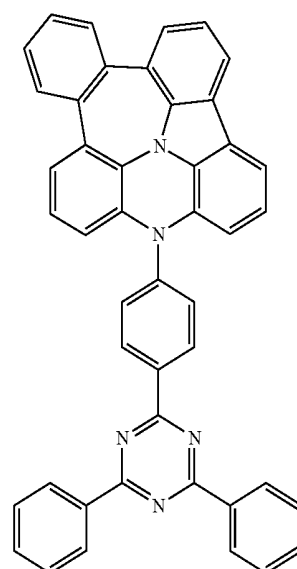
[0078] Element analysis: (C₄₅H₂₉N₅) calculated: C, 84.48; H, 4.57; N, 10.95. found: C, 84.50; H, 4.55; N, 10.96, HRMS (ESI) *m/z* (M⁺): calculated: 639.24. found: 639.27.

Example 3

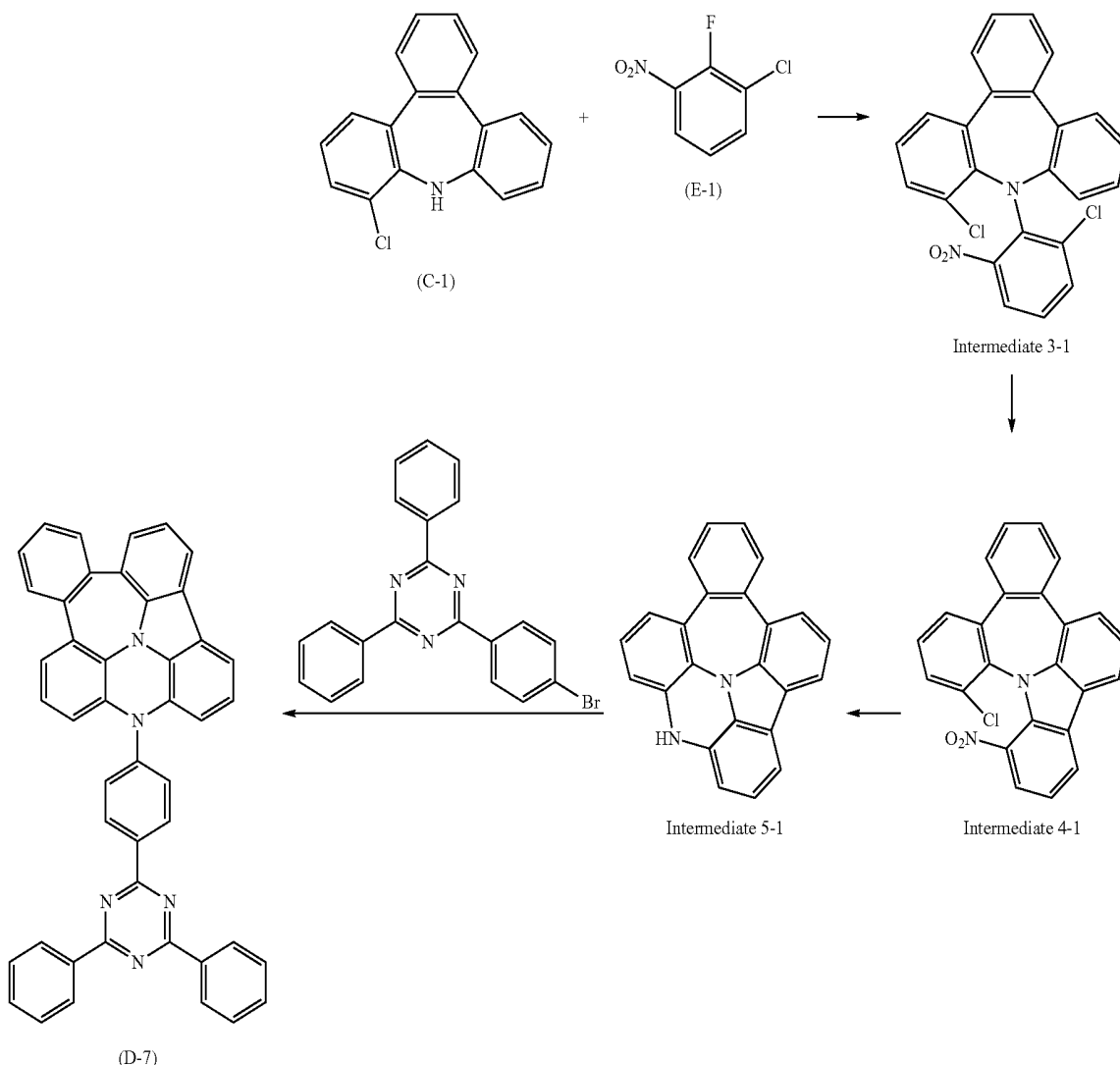
[0079] This example provides a fused cyclic compound having a structure of Formula D-7 below:



2 g 5.1 mmol), sodium-*t*-butoxide (1.41 g), and toluene (750 mL) were added, reacted at 110° C. for 12 hrs, and then cooled to room temperature. The reaction solution was extracted with chloroform, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain a solid compound C-16 (2.6 g, yield 81%).



[0080] The synthesis route for the fused cyclic compound of Formula D-7 is shown below:



[0081] The method for preparing the fused cyclic compound of Formula D-7 comprises specifically the following steps.

(1) Synthesis of Intermediate 3-1

[0082] Under nitrogen atmosphere, a compound of Formula (C-1) (5.6 g, 20 mmol), 3-chloro-2-fluoronitrobenzene (a compound of Formula (E-1)) (3.5 g, 20 mmol), cesium carbonate (7.8 g, 24 mmol), and dimethyl sulfoxide (80 mL) were added to a 500 mL three-neck flask, and reacted for 15 hrs. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 3-1 as a solid (6.5 g, yield 75%).

(2) Synthesis of Intermediate 4-1

[0083] Under nitrogen atmosphere, the intermediate 3-1 (4.3 g, 10 mmol), palladium diacetate (0.2 g, 1.0 mmol),

tricyclohexylphosphonium tetrafluoroborate (0.73 g, 2.0 mmol), cesium carbonate (9.7 g, 30 mmol), and o-xylene (50 mL) were added, and reacted under reflux with heating for 2 hrs. The reaction solution was extracted with chloroform, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 4-1 as a solid (2.8 g, yield 75%).

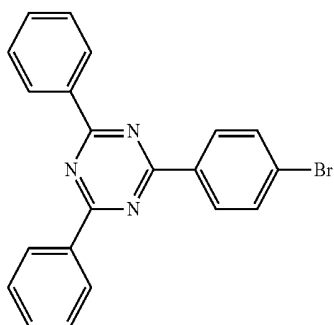
(3) Synthesis of Intermediate 5-1

[0084] Under nitrogen atmosphere, the intermediate 4-1 (2.8 g, 7 mmol), stannous chloride dihydrate (6.3 g, 28 mmol), hydrochloric acid (5 mL), and ethanol (40 mL) were added, and reacted for 10 hrs at 60° C. The reaction solution was extracted with chloroform, washed with water and then with brine, and dried over anhydrous magnesium sulfate, and then the solvent was removed by rotary evaporation. After drying, the residue was transferred to a reaction flask, and tris(dibenzylideneacetone)dipalladium (64 mg, 0.07

mmol) and toluene (50 mL) were added, reacted for 8 hrs at 110° C., and then cooled to room temperature. The reaction solution was extracted with chloroform and washed with water, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 5-1 as a solid (1.68 g, yield 71%).

(4) Synthesis of Fused Cyclic Compound D-7

[0085] Under nitrogen atmosphere, the intermediate 5-1 (1.65 g, 5 mmol), palladium diacetate (0.03 g, 0.15 mmol), tri-tert-butylphosphine (0.1 g, 0.55 mmol), the compound



(2 g 5.1 mmol), sodium-t-butoxide (1.41 g), and toluene (750 mL) were added, reacted at 110° C. for 12 hrs, and then cooled to room temperature. The reaction solution was extracted with chloroform, and then the solvent was

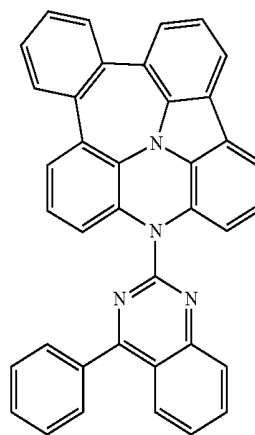
removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the fused cyclic compound D-7 as a solid (2.5 g, yield 79%).

[0086] Element analysis: (C₄₅H₂₇N₅) calculated: C, 84.75; H, 4.27; N, 10.98. found: C, 84.78; H, 4.25; N, 11.01. HRMS (ESI) m/z (M⁺): calculated: 637.23. found: 637.41.

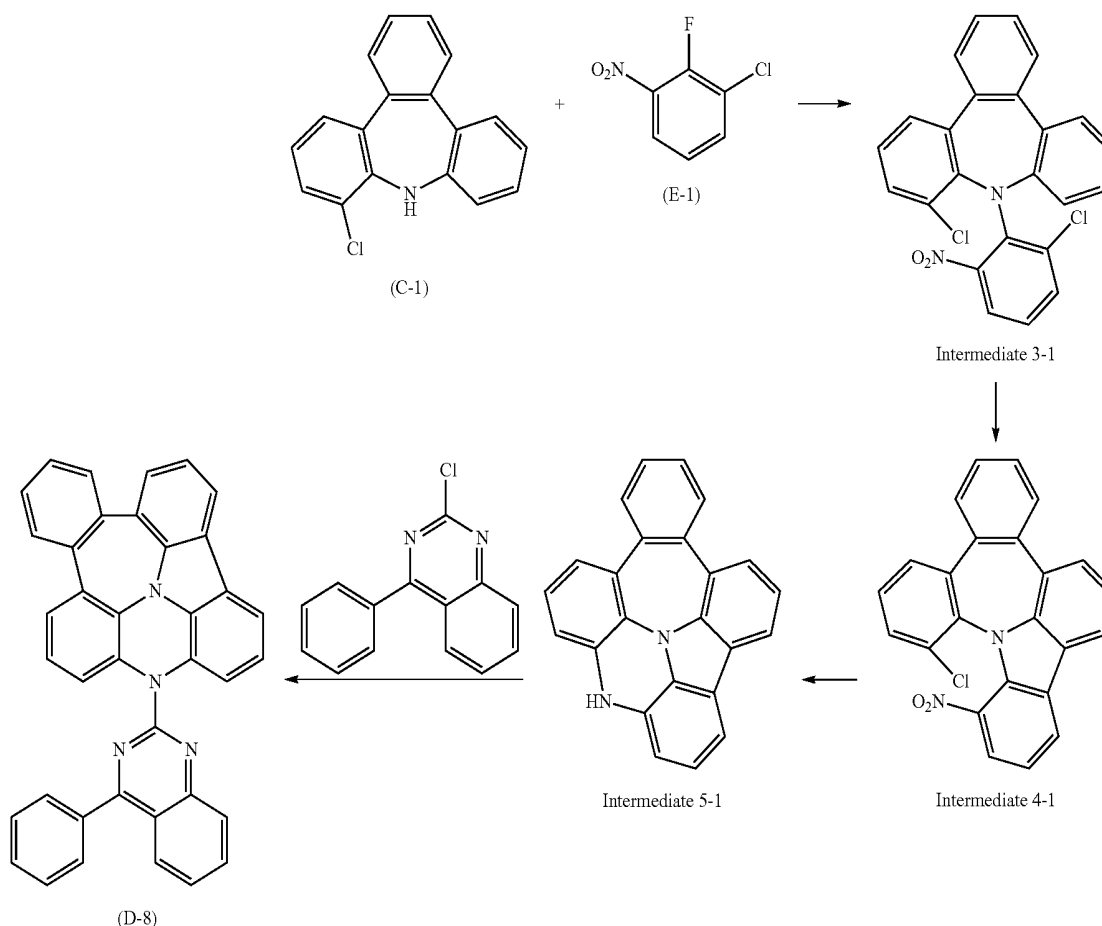
Example 4

[0087] This example provides a fused cyclic compound having a structure of Formula D-8 below:

(D-8)



[0088] The synthesis route for the fused cyclic compound of Formula D-8 is shown below:

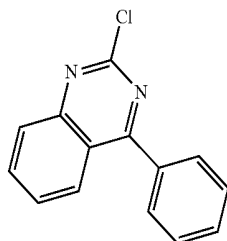


[0089] The method for preparing the fused cyclic compound of Formula D-8 comprises specifically the following steps.

[0090] (1) The intermediate 5-1 was synthesized following the method as described in Example 3.

[0091] (2) Synthesis of Fused Cyclic Compound D-8

[0092] Under nitrogen atmosphere, the intermediate 5-1 (1.65 g, 5 mmol), the compound

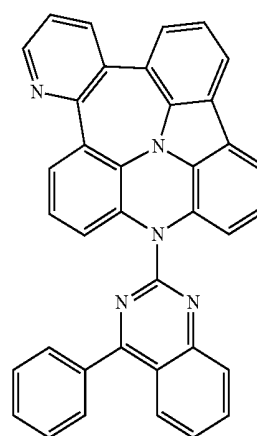


(1.6 g, 6 mmol), cesium carbonate (1.7 g, 5 mmol), 4-dimethylamino pyridine (0.3 g, 2.5 mmol), and dimethyl sulfoxide (20 mL) were added, reacted at 100° C. for 3 hrs, and then cooled to room temperature. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the compound D-8 as a solid (2.2 g, yield 83%).

[0093] Element analysis: (C₃₈H₂₂N₄) calculated: C, 85.37; H, 4.15; N, 10.48. found: C, 85.34; H, 4.21; N, 10.53, HRMS (ESI) m/z (M⁺): calculated: 534.18. found: 534.32.

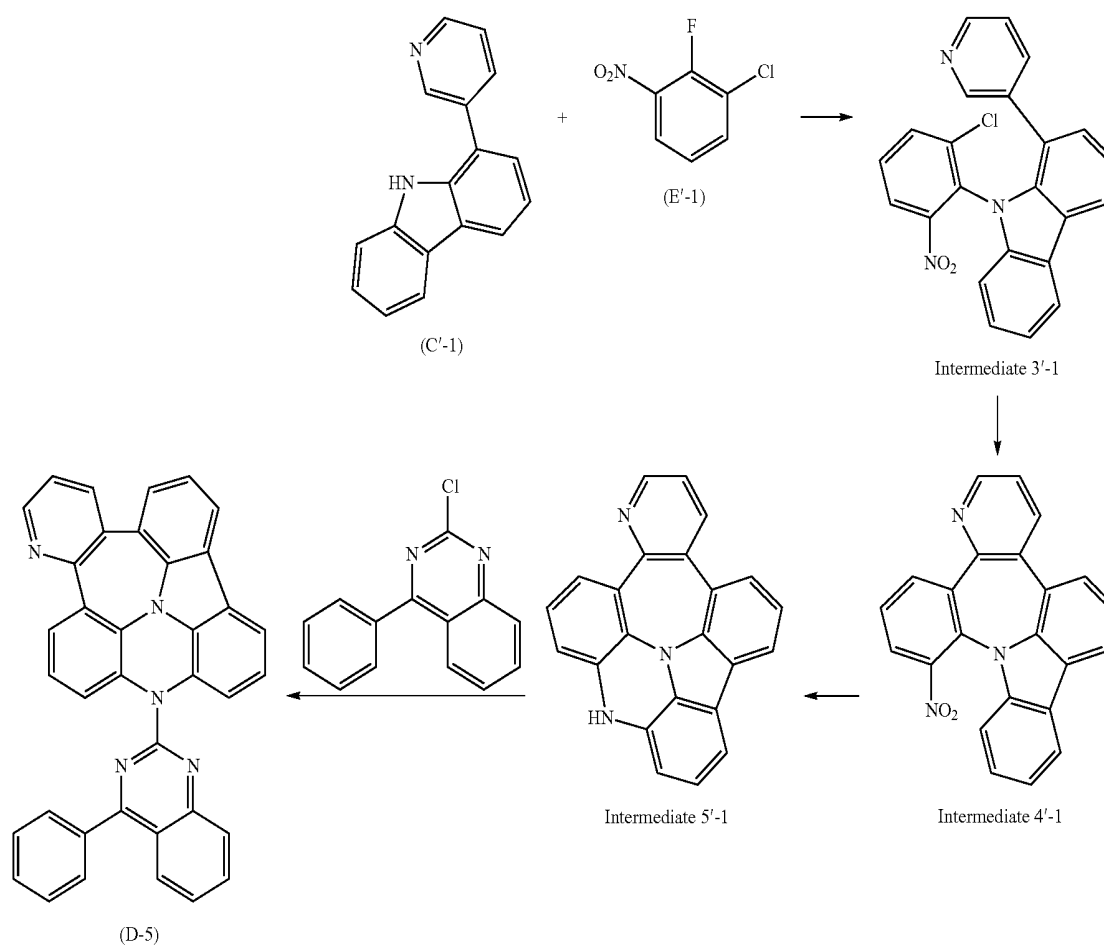
Example 5

[0094] This example provides a fused cyclic compound having a structure of Formula D-5 below:



(D-5)

[0095] The synthesis route for the fused cyclic compound of Formula D-5 is shown below:



[0096] The method for preparing the fused cyclic compound of Formula D-5 comprises specifically the following steps.

(1) Synthesis of Intermediate 3'-1

[0097] Under nitrogen atmosphere, a compound of Formula (C'-1) (12.2 g, 50 mmol), 3-chloro-2-fluoronitrobenzene (8.8 g, 50 mmol) (a compound of Formula (E'-1)), cesium carbonate (19.5 g, 60 mmol), and dimethyl sulfoxide (200 mL) were added to a 500 mL three-neck flask, and reacted for 15 hrs. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 3'-1 as a solid (14.3 g, yield 72%).

(2) Synthesis of Intermediate 4'-1

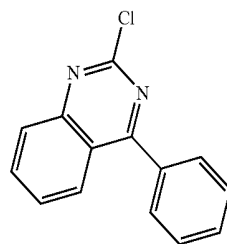
[0098] Under nitrogen atmosphere, the intermediate 3'-1 (12 g, 30 mmol), palladium diacetate (0.6 g, 3.0 mmol), tricyclohexylphosphonium tetrafluoroborate (2.2 g, 6.0 mmol), cesium carbonate (29.1 g, 90 mmol), and o-xylene (150 mL) were added, and reacted under reflux with heating for 2 hrs. The reaction solution was extracted with chloroform, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 4'-1 as a solid (8.2 g, yield 75%).

(3) Synthesis of Intermediate 5'-1

[0099] Under nitrogen atmosphere, the intermediate 4'-1 (7.6 g, 21 mmol), stannous chloride dihydrate (18.9 g, 84 mmol), hydrochloric acid (15 mL), and ethanol (120 mL) were added, and reacted for 10 hrs at 60° C. The reaction solution was extracted with chloroform, washed with water and then with brine, and dried over anhydrous magnesium sulfate, and then the solvent was removed by rotary evaporation. After drying, the residue was transferred to a reaction flask, and tris(dibenzylideneacetone)dipalladium (0.19 g, 0.21 mmol) and toluene (150 mL) were added, reacted for 8 hrs at 110° C., and then cooled to room temperature. The reaction solution was extracted with chloroform and washed with water, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain the intermediate 5'-1 as a solid (5.13 g, yield 73%).

(4) Synthesis of Fused Cyclic Compound D-5

[0100] Under nitrogen atmosphere, the intermediate 5'-1 (3.3 g, 10 mmol), the compound

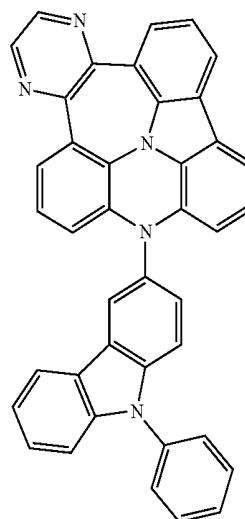


(3.2 g, 12 mmol), cesium carbonate (3.4 g, 10 mmol), 4-dimethylamino pyridine (0.6 g, 5.0 mmol), and dimethyl sulfoxide (40 mL) were added, reacted at 100° C. for 3 hrs, and then cooled to room temperature. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain a fused cyclic compound D-5 (4.6 g, yield 85%).

[0101] Element analysis: (C₃₇H₂₃N₅) calculated: C, 82.66; H, 4.31; N, 13.03. found: C, 82.68; H, 4.28; N, 13.01, HRMS (ESI) m/z (M⁺): calculated: 537.20. found: 535.27.

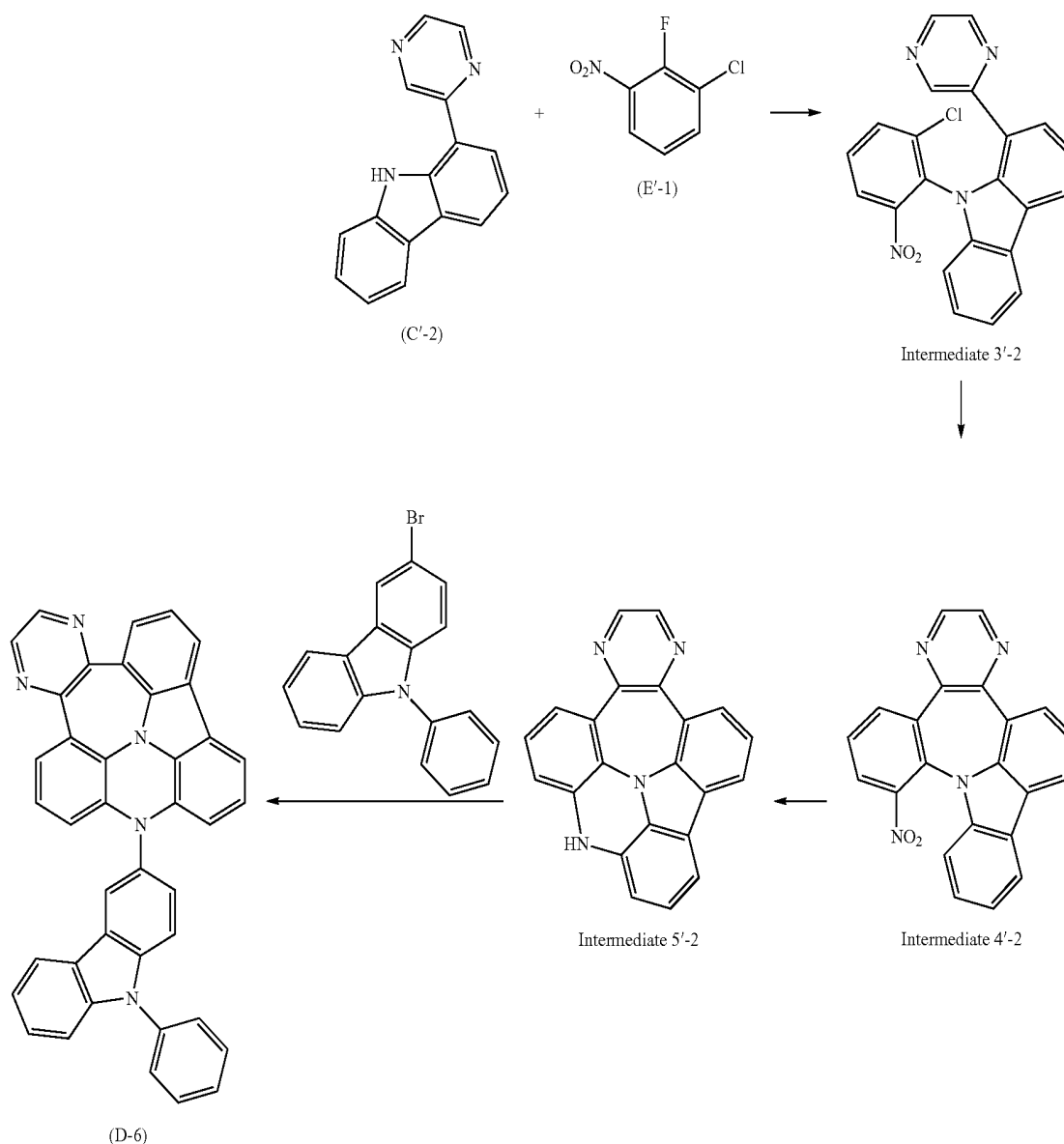
Example 6

[0102] This example provides a fused cyclic compound having a structure of Formula D-6 below:



(D-6)

[0103] The synthesis route for the fused cyclic compound of Formula D-6 is shown below:

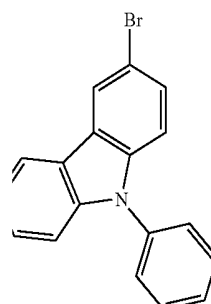


[0104] The method for preparing the fused cyclic compound of Formula D-6 comprises specifically the following steps.

[0105] (1) Starting with the compound of Formula (C'-2) and the compound of Formula (E'-1), the intermediate 5'-2 was synthesized following the synthesis method in Example 5.

[0106] (2) Synthesis of Fused Cyclic Compound D-6

[0107] Under nitrogen atmosphere, the intermediate 5'-1 (5.6 g, 16.7 mmol), the compound



(5.5 g, 17 mmol), palladium diacetate (0.11 g, 0.5 mmol), tri-tert-butylphosphine (0.37 g, 1.83 mmol), sodium-t-butoxide (4.7 g), and toluene (250 mL) were added, reacted at 110° C. for 12 hrs, and cooled to room temperature. The reaction solution was extracted with toluene, and then the solvent was removed by rotary evaporation. The residue was purified by column chromatography on silica gel, to obtain a fused cyclic compound D-6 (8.2 g, yield 85%).

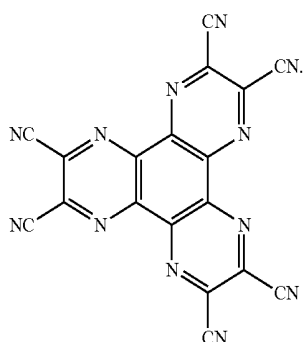
[0108] Element analysis: (C₄₀H₂₅N₅) calculated: C, 83.46; H, 4.38; N, 12.17. found: C, 83.42; H, 4.41; N, 12.14. HRMS (ESI) m/z (M⁺): calculated: 575.21. found: 575.27.

Example 7

[0109] This example provides an organic light-emitting device, which includes, from bottom to top, an anode **2**, a hole injection layer **1**, a hole transport layer **3**, a light emitting layer **4**, an electron transport layer **5**, an electron injection layer **6** and a cathode **7** stacked in sequence, as shown in FIG. 2.

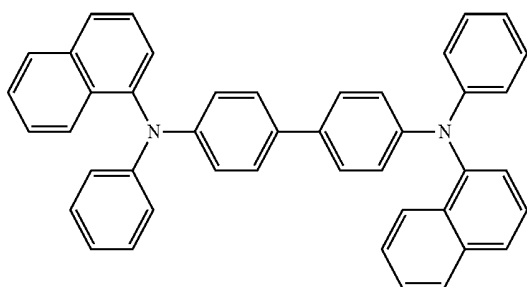
[0110] In the organic light-emitting device, the material of the anode is ITO; and the material of the cathode **7** is the metal Al.

[0111] The material of the hole injection layer **2** is HAT (CN)₆, having a chemical structure as shown below:

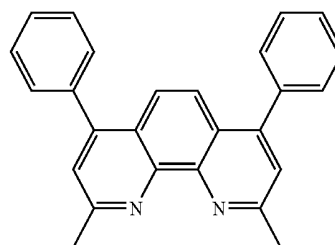


HAT(CN)₆

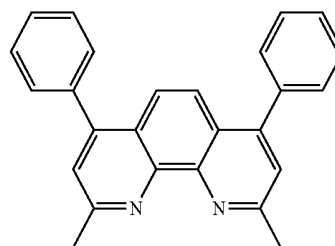
[0112] The material of the hole transport layer **3** is a compound having a structure below:



[0113] The material of the electron transport layer **5** is a compound having a structure below:

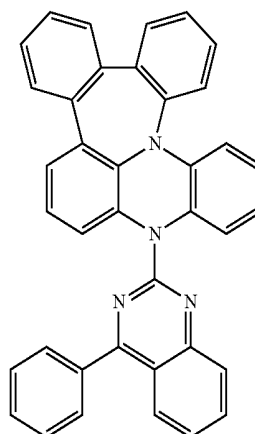


[0114] The material of the electron injection layer **6** is formed by a compound having a structure below, blended with the electron injection material LiF:

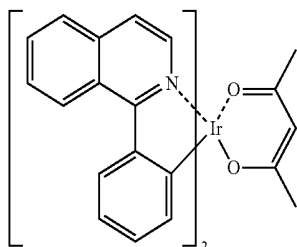


[0115] In the organic light-emitting device, the light emitting layer **32** is formed by blending a host material and a guest luminescent dye, where the host material is the fused cyclic compound (D-2), and the guest material is the compound RD, and the host material and the guest material are blended at a weight ratio of 100:5. The organic light-emitting device is configured to have a particular structure of ITO/hole injection layer (HIL)/hole transport layer (HTL)/organic light emitting layer (fused cyclic compound D-2 blended with compound RD)/electron transport layer (ETL)/electron injection layer (EIL/LiF)/cathode (Al). The fused cyclic compound (D-2), and the compound RD have the following chemical structures:

(D-2)

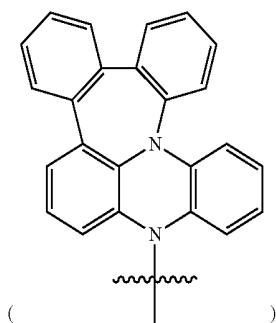


-continued



RD

[0116] The host material in the light-emitting layer is the fused cyclic compound of Formula D-2, which has increased effective conjugation in the compound by the fusion mode of the phenyl ring and the heterocyclic ring in the mother nuclear structure, and facilitates the balancing of the electron transport performance while improving the hole performance of the compound. The fused cyclic compound of D-2 has high triplet energy level and glass transition temperature, which ensures the efficient transfer of energy from the host material to the guest material and prevents the crystallization of the material molecules of the light emitting layer. Meanwhile, the compound has ambipolarity, the HOMO level and the LUMO level of the host material are respectively located on different electron donating group



and electron withdrawing group (quinazoline), and the transport of charges and holes in the host material becomes more balanced, thereby expanding the area where holes and electrons are recombined into excitons in the light emitting layer, reducing the exciton concentration, preventing the triplet-triplet annihilation of the device, and improving the efficiency of the device; and also the carrier recombination region in the host material is allowed to stay far away from the interface of the light emitting layer to the hole or electron transport layer, thus improving the color purity of the OLED device, avoiding the returning of excitons to the transport layer, and further improving the efficiency of the device.

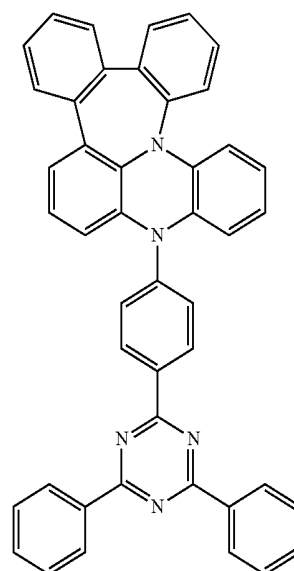
[0117] The HOMO level and the LUMO level of the fused cyclic compound D-2 match those of the adjacent hole transport layer and electron transport layer, so that the OLED device has a small driving voltage.

[0118] The HOMO level and the LUMO level of the fused cyclic compound D-2 are relatively separated, with a small difference (ΔE_{ST}) between singlet and triplet energy levels, which promotes the reverse intersystem crossing of triplet excitons to singlet excitons. Moreover, the high reverse intersystem crossing (RISC) rate from the triplet state T1 to the singlet state S1 of the host material can suppress the Dexter energy transfer (DET) from the host material to the luminescent dye, promote the Föster energy transfer, reduce the exciton loss generated during the Dexter energy transfer (DET), thus avoiding the efficiency roll-off of the organic light-emitting device and improving the luminescence efficiency of the device.

[0119] In an alternative embodiment, the host material in the light emitting layer may also be any fused cyclic compound of Formulas (D-1)-(D-21).

Example 8

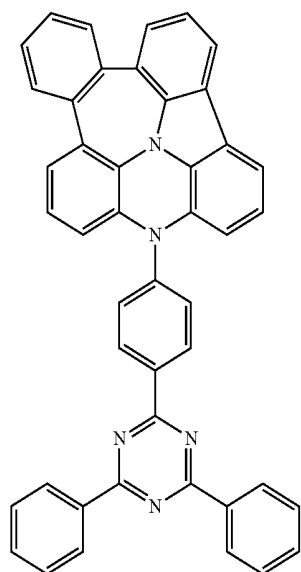
[0120] This example provides an organic light-emitting device, which differs from the organic light-emitting device provided in Embodiment 7 only in that the host material in the light emitting layer is a fused heterocyclic compound having a structure shown below:



(D-1)

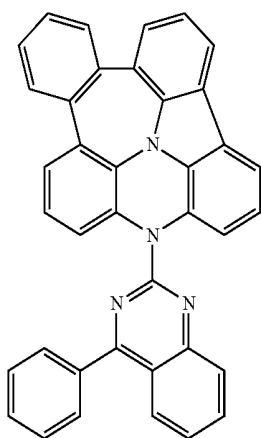
Example 9

[0121] This example provides an organic light-emitting device, which differs from the organic light-emitting device provided in Embodiment 7 only in that the host material in the light emitting layer is a fused heterocyclic compound having a structure shown below:



Example 10

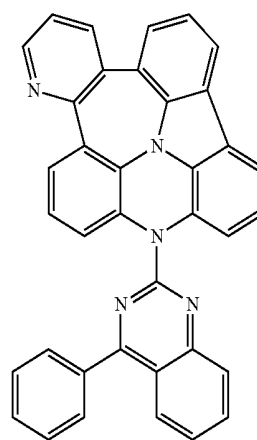
[0122] This example provides an organic light-emitting device, which differs from the organic light-emitting device provided in Embodiment 7 only in that the host material in the light emitting layer is a fused heterocyclic compound having a structure shown below:



Example 11

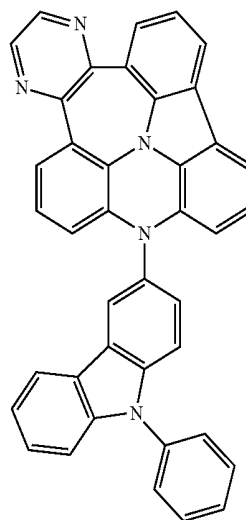
[0123] This example provides an organic light-emitting device, which differs from the organic light-emitting device provided in Embodiment 7 only in that the host material in the light emitting layer is a fused heterocyclic compound having a structure shown below:

(D-7)



Example 12

[0124] This example provides an organic light-emitting device, which differs from the organic light-emitting device provided in Embodiment 7 only in that the host material in the light emitting layer is a fused heterocyclic compound having a structure shown below:



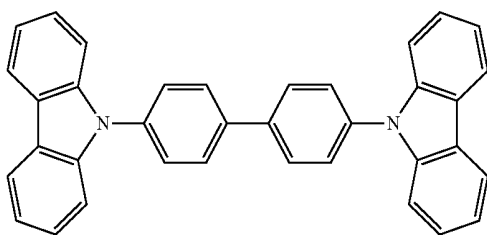
Comparative Example 1

[0125] This comparative example provides an organic light-emitting device, which differs from the organic light-emitting device provided in Embodiment 7 only in that the host material in the light emitting layer is 4,4'-bis(9-carbazole)biphenyl (CBP).

(D-5)

(D-8)

(D-6)



Test Example 1

[0126] 1. Determination of Glass Transition Temperature

[0127] The glass transition temperature of the material according to the present invention was tested by differential scanning calorimetry (DSC) in a range from room temperature to 400° C. at a ramping rate of 10° C./min under nitrogen atmosphere.

[0128] 2. The fluorescence and phosphorescence spectra of a solution of the fused heterocyclic compound in toluene (having a concentration of 10^{-5} mol/L) were measured at 298 K and 77 K, respectively, the corresponding singlet (S1) and triplet (T1) energy levels were calculated according to the formula $E=1240/\lambda$, and then a difference between the singlet and triplet energy levels of the fused heterocyclic compound was obtained. The difference between the energy levels of the fused heterocyclic compound is shown below.

TABLE 1

Fused Heterocyclic Compound	Formula D-2	Formula D-1	Formula D-7	Formula D-8	Formula D-5	Formula D-6
Glass Transition Temperature (° C.)	158	162	169	161	160	165
T1 (eV)	2.74	2.72	2.67	2.70	2.65	2.68
S1-T1 (eV)	0.25	0.19	0.17	0.21	0.14	0.30

Test Example 2

[0129] The current, voltage, brightness, and luminescence spectrum of the device were tested synchronously using PR 650 scanning spectroradiometer and Keithley K 2400 digital source meter. The organic light-emitting devices provided in Examples 7-12 and Comparative Example 1 were tested. The results are shown in Table 2.

TABLE 2

	Host material	Voltage/V	Current density/ mA/cm ²	Current efficiency cd/A	Chromaticity (CIE-X, Y)
Comparative Example 1	CBP	5.1	10	21	(0.66, 0.33)
Example 7	D-2	4.1	10	27	(0.66, 0.33)
Example 8	D-1	3.8	10	24	(0.66, 0.33)
Example 9	D-7	3.7	10	24	(0.66, 0.33)
Example 10	D-8	4.0	10	28	(0.66, 0.33)
Example 11	D-5	3.2	10	23	(0.66, 0.33)
Example 12	D-6	3.5	10	24	(0.66, 0.33)

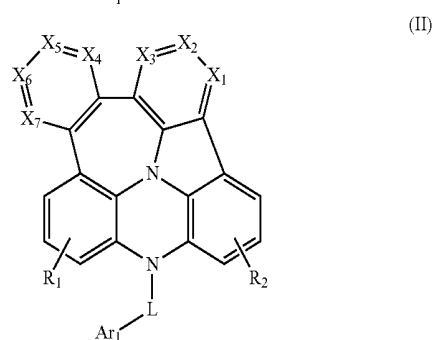
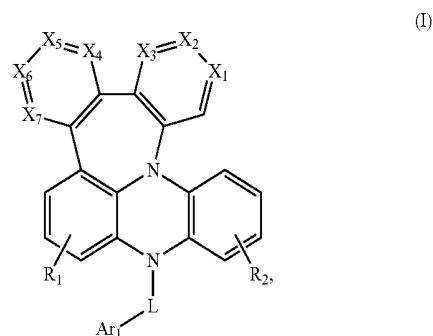
[0130] The organic light-emitting devices provided in Examples 7-12 and Comparative Example 1 were tested.

The results are shown in Table 2. The luminescence efficiency of the OLED devices provided in Examples 7-12 is higher than that of the OLED device in Comparative Example 1, and the driving voltage is lower than that of the OLED device in Comparative Example 1, indicating that the fused heterocyclic compound provided in the present invention, when used as a host material in a light emitting layer of an OLED device, can effectively improve the luminescence efficiency and reduce the driving voltage of the device.

[0131] Apparently, the above-described embodiments are merely examples provided for clarity of description, and are not intended to limit the implementations of the present invention. Other variations or changes can be made by those skilled in the art based on the above description. The embodiments are not exhaustive herein. Obvious variations or changes derived therefrom also fall within the protection scope of the present invention.

What is claimed is:

1. A fused cyclic compound, having a structure of Formula (I) or (II):



wherein X_1 is selected from N or C— R_{1a} , X_2 is selected from N or C— R_{2a} , X_3 is selected from N or C— R_{3a} , X_4 is selected from N or C— R_{4a} , X_5 is selected from N or C— R_{5a} , X_6 is selected from N or C— R_{6a} , and X_7 is selected from N or C— R_{7a} , in which

R_{1a} - R_{7a} are each independently selected from hydrogen, halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, silyl, aryl or heteroaryl;

R_1 , and R_2 are each independently selected from hydrogen, halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, silyl, aryl or heteroaryl;

L is a single bond, a C_1 - C_{10} substituted or unsubstituted aliphatic hydrocarbon group, a C_6 - C_{60} substituted or unsubstituted aryl group, or a C_3 - C_{30} substituted or unsubstituted heteroaryl group; and

Ar_i is selected from hydrogen, halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, silyl, aryl or heteroaryl, in which

the heteroaryl has at least one heteroatom independently selected from nitrogen, sulfur, oxygen, phosphorous, boron or silicon.

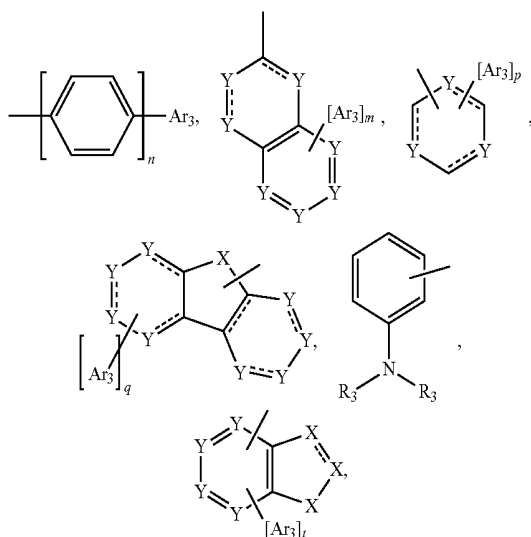
2. The fused cyclic compound according to claim 1, wherein

R_1 and R_2 are each independently selected from hydrogen, halo, cyano, a C_1 - C_{30} substituted or unsubstituted alkyl group, a C_2 - C_{30} substituted or unsubstituted alkenyl group, a C_2 - C_{30} substituted or unsubstituted alkynyl group, a C_3 - C_{30} substituted or unsubstituted cycloalkyl group, a C_1 - C_{30} substituted or unsubstituted alkoxy group, a C_1 - C_{30} substituted or unsubstituted silyl group, a C_6 - C_{60} substituted or unsubstituted aryl group, or a C_3 - C_{30} substituted or unsubstituted heteroaryl group;

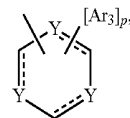
Ar_1 is selected from hydrogen, halo, cyano, a C_1 - C_{30} substituted or unsubstituted alkyl group, a C_2 - C_{30} substituted or unsubstituted alkenyl group, a C_2 - C_{30} substituted or unsubstituted alkynyl group, a C_3 - C_{30} substituted or unsubstituted cycloalkyl group, a C_1 - C_{30} substituted or unsubstituted alkoxy group, a C_1 - C_{30} substituted or unsubstituted silyl group, a C_6 - C_{60} substituted or unsubstituted aryl group, or a C_3 - C_{30} substituted or unsubstituted heteroaryl group; and

R_{1a} - R_{7a} are each independently selected from hydrogen, halo, cyano, a C_1 - C_{30} substituted or unsubstituted alkyl group, a C_2 - C_{30} substituted or unsubstituted alkenyl group, a C_2 - C_{30} substituted or unsubstituted alkynyl group, a C_3 - C_{30} substituted or unsubstituted cycloalkyl group, a C_1 - C_{30} substituted or unsubstituted alkoxy group, a C_1 - C_{30} substituted or unsubstituted silyl group, a C_6 - C_{60} substituted or unsubstituted aryl group, or a C_3 - C_{30} substituted or unsubstituted heteroaryl group.

3. The fused cyclic compound according to claim 1, wherein Ar_1 is selected from any of the following groups, and R_1 , R_2 , R_{1a} , R_{2a} , R_{3a} , R_{4a} , R_{5a} , R_{6a} , and R_{7a} are each independently selected from hydrogen or any of the following groups:



where X is nitrogen, oxygen or sulfur, Y is each independently nitrogen or carbon; and in the



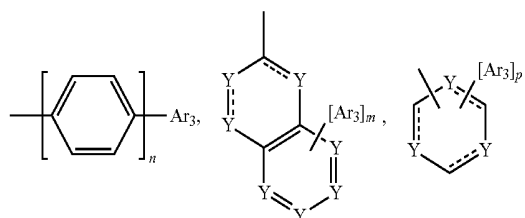
at least one Y is nitrogen; and

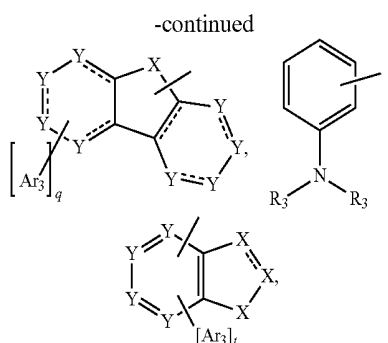
n is an integer of 0-5, m is an integer of 0-7, p is an integer of 0-6, q is an integer of 0-8, and t is an integer of 0-7; and ----- is a single or double bond;

R_3 is each independently selected from a substituted or unsubstituted phenyl group or hydrogen; and

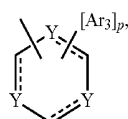
Ar_3 is each independently selected from hydrogen, phenyl, coronenyl, pentalenyl, indenyl, naphthyl, azulenyl, fluorenyl, heptalenyl, octalenyl, benzodiindenyl, acenaphthylenyl, phenalenyl, phenanthrenyl, anthracenyl, triindenyl, fluoranthrenyl, benzopyrenyl, benzoperylenyl, benzofluoranthrenyl, acephenanthrenyl, aceanthrylenyl, 9,10-benzophenanthrenyl, pyrenyl, 1,2-benzophenanthrenyl, butylphenyl, naphthacenyl, pleiadenyl, picenyl, perylenyl, pentaphenyl, pentaceny, tetraphenylene, cholanthrenyl, helicenyl, hexaphenyl, rubicenyl, coronenyl, trinaphthylenyl, heptaphenyl, pyranthrenyl, ovalenyl, corannulenyl, anthanthrenyl, truxenyl, pyranyl, benzopyranyl, furyl, benzofuryl, isobenzofuryl, oxanthracenyl, oxazolynyl, dibenzofuryl, peri-xanthenoxanthrenyl, thienyl, thioxanthrenyl, thianthrenyl, phenoxathiynyl, thionaphthenyl, isothionaphthenyl, thiophanthrenyl, dibenzothieryl, benzothieryl, pyrrolyl, pyrazolyl, tellurazolyl, selenazolyl, thiazolyl, isothiazolyl, oxazolyl, oxadiazolyl, furazanyl, pyridinyl, pyrazinyl, pyrimidinyl, pyridazinyl, triazinyl, indolizynyl, indolyl, isoindolyl, indazolyl, purinyl, quinolizynyl, isoquinolyl, carbazolyl, fluoreno-carbazolyl, indolocarbazolyl, imidazolyl, naphthyridinyl, phthalazinyl, quinazolynyl, benzodiazepinyl, quinoxalinyl, cinnolinyl, quinolyl, pteridinyl, phenanthridinyl, acridinyl, perimidinyl, phenanthroli-nyl, phenazinyl, carbolinyl, phenotellurazinyl, phenoselenazinyl, phenothiazinyl, phenoxazinyl, triphenodithiazinyl, azadibenzofuryl, triphenodioxazinyl, anthrazinyl, benzothiazolyl, benzoimidazolyl, benzoxazolyl, benzisoxazolyl or benzoisothiazolyl.

4. The fused cyclic compound according to claim 2, wherein Ar_i is selected from any of the following groups, and R_1 , R_2 , R_{1a} , R_{2a} , R_{3a} , R_{4a} , R_{5a} , R_{6a} , and R_{7a} are each independently selected from hydrogen or any of the following groups:





where X is nitrogen, oxygen or sulfur, Y is each independently nitrogen or carbon; and in the

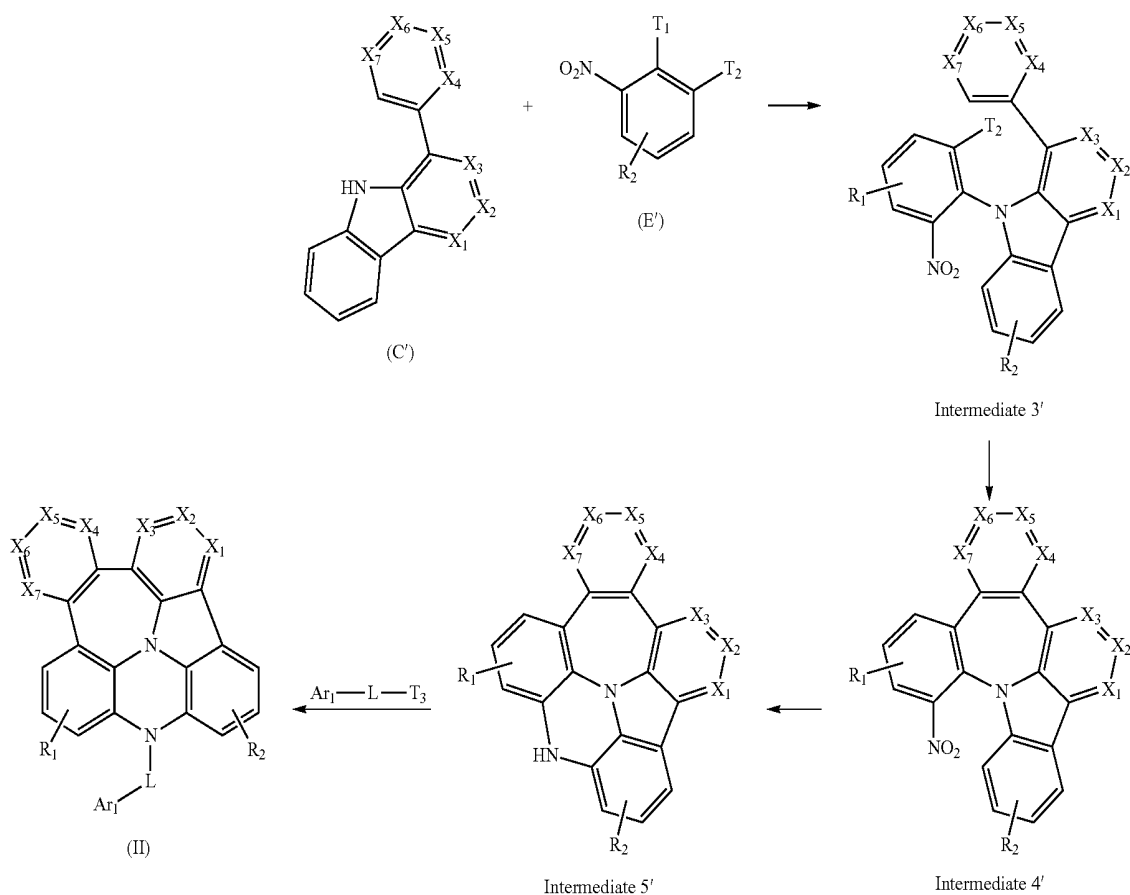


at least one Y is nitrogen; and

n is an integer of 0-5, m is an integer of 0-7, p is an integer of 0-6, q is an integer of 0-8, and t is an integer of 0-7; and --- is a single or double bond;

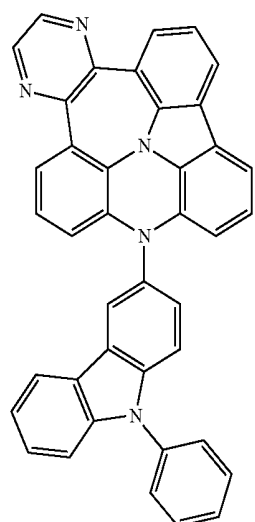
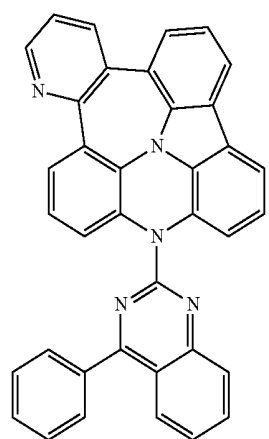
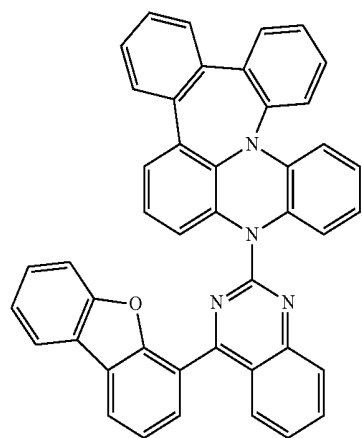
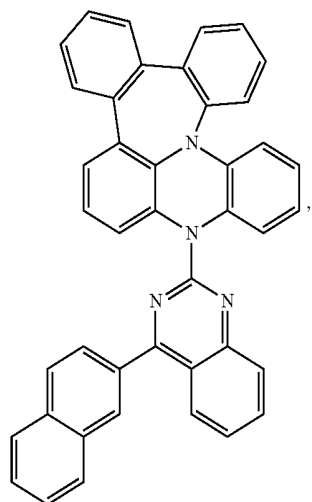
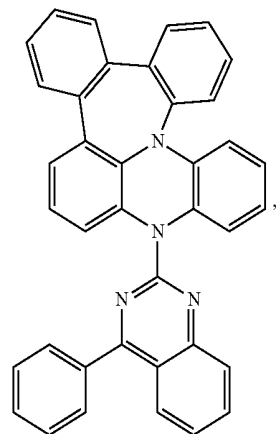
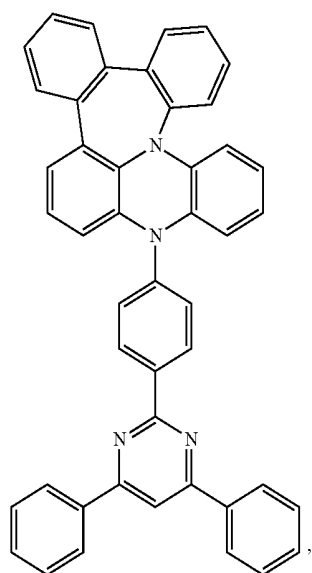
R_3 is each independently selected from a substituted or unsubstituted phenyl group or hydrogen; and

Ar_3 is each independently selected from hydrogen, phenyl, coronenyl, pentalenyl, indenyl, naphthyl, azulenyl, fluorenyl, heptalenyl, octalenyl, benzodiindenyl, acenaphthyl, phenalenyl, phenanthrenyl, anthracenyl, triindenyl, fluoranthrenyl, benzopyrenyl, benzoperylenyl, benzofluoranthrenyl, acephenanthrenyl, aceanthrylenyl, 9,10-benzophenanthrenyl, pyrenyl, 1,2-benzophenanthrenyl, butylphenyl, naphthacenyl, pleiadenyl, picenyl, perylenyl, pentaphenyl, pentacenyl, tetraphenylene, cholanthrenyl, helicenyl, hexaphe-nyl, rubicenyl, coronenyl, trinaphthyl, heptaphe-nyl, pyranthrenyl, ovalenyl, corannulenyl, anthanthrenyl, truxenyl, pyranyl, benzopyranyl, furyl, benzofuryl, isobenzofuryl, oxanthracenyl, oxazolinyl, dibenzofuryl, peri-xanthenoxanthrenyl, thienyl, thioxanthrenyl, thianthrenyl, phenoxathiinyl, thionaphthyl, isothionaphthyl, thiophanthrenyl, dibenzothieryl, benzothieryl, pyrrolyl, pyrazolyl, tellurazolyl, selenazolyl, thiazolyl, isothiazolyl, oxazolyl, oxadiazolyl, furazanyl, pyridinyl, pyrazinyl, pyrimidinyl, pyridazinyl, triazinyl, indoliziny, indolyl, isoindolyl, indazolyl, purinyl, quinoliziny, isoquinolyl, carbazolyl, fluoreno-carbazolyl, indolocarbazolyl, imidazolyl, naphthyridinyl, phthalazinyl, quinazolinyl, benzodiazepinyl, quinoxalinyl, cinnoliny, quinolyl, pteridinyl, phenanthridinyl, acridinyl, perimidinyl, phenanthroli-nyl, phenaziny, carbolinyl, phenotellurazinyl, phenoselenazinyl, phenothiazinyl, phenoxazinyl, tripheno-dithiazinyl, azadibenzofuryl, triphenodioxazinyl, anthrazinyl, benzothiazolyl, benzoimidazolyl, benzox-azolyl, benzisoxazolyl or benzoisothiazolyl.



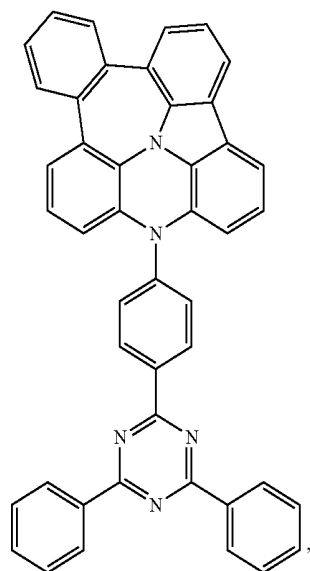
where T₁-T₅ are each independently selected from hydrogen, fluoro, chloro, bromo or iodo.

5. The fused cyclic compound according to claim 1, having a molecular structure shown below:

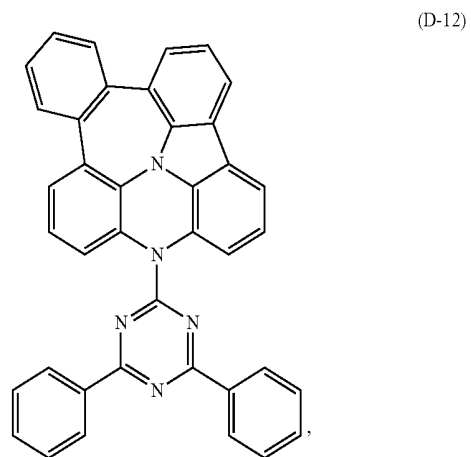
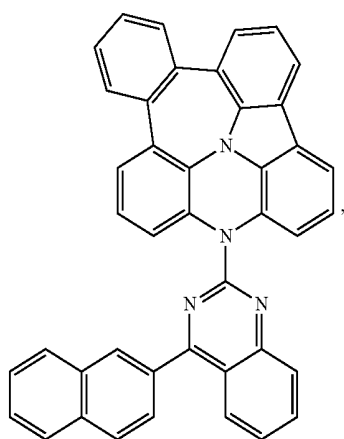
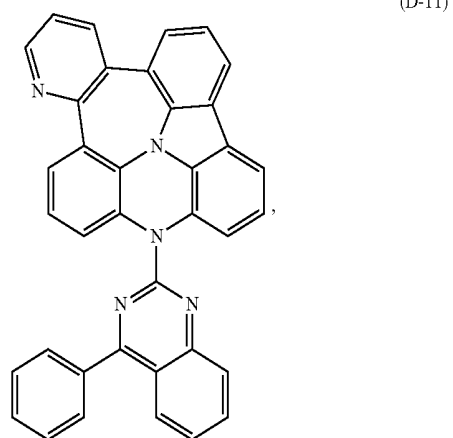
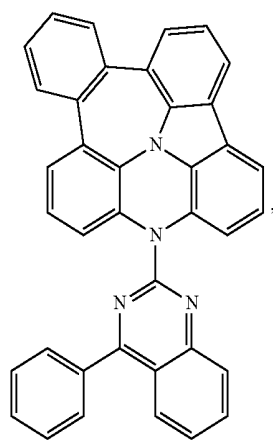
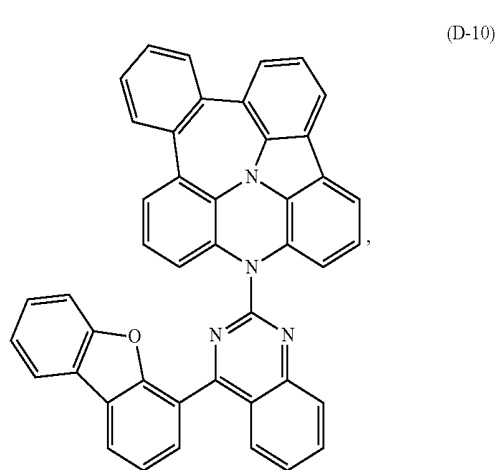


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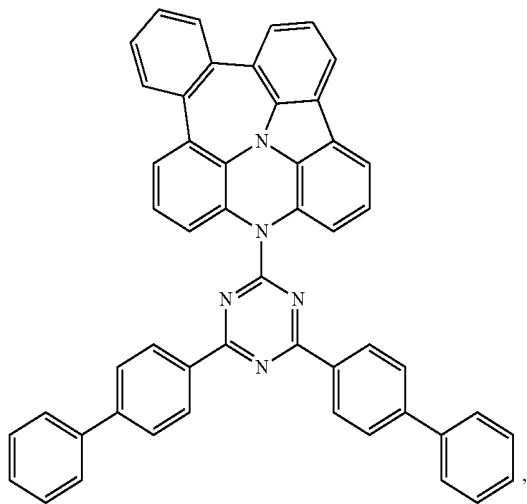


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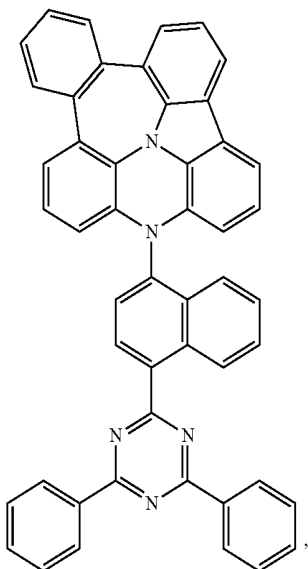


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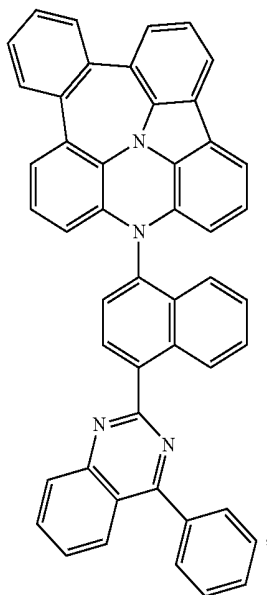
(D-13)



(D-14)

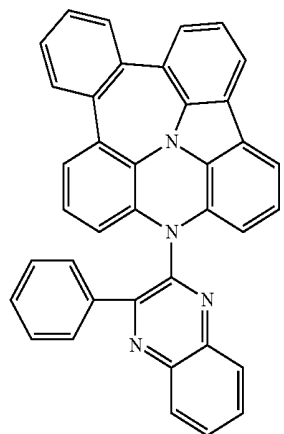


(D-15)

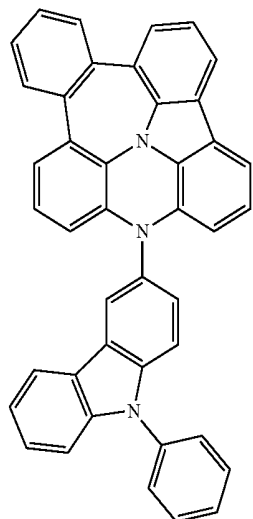


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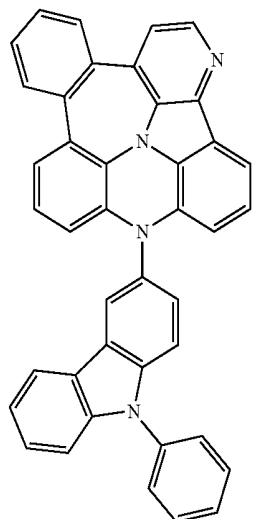
(D-16)



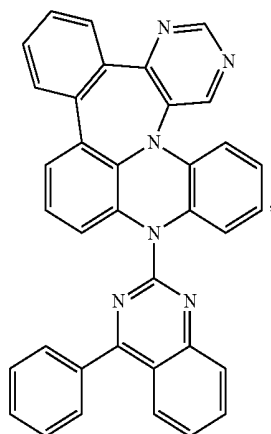
(D-17)



(D-18)



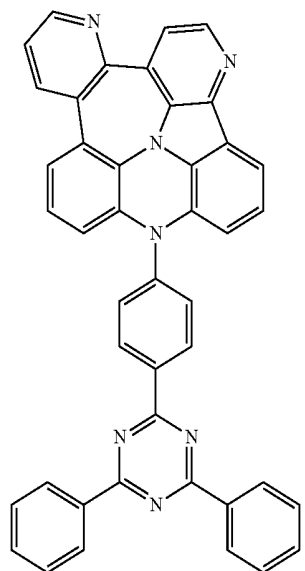
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(D-19)

-continued

(D-21)



6. The fused cyclic compound according to claim 1, wherein the fused cyclic compound is an organic electroluminescent material.

7. The fused cyclic compound according to claim 2, wherein the fused cyclic compound is an organic electroluminescent material.

8. The fused cyclic compound according to claim 3, wherein the fused cyclic compound is an organic electroluminescent material.

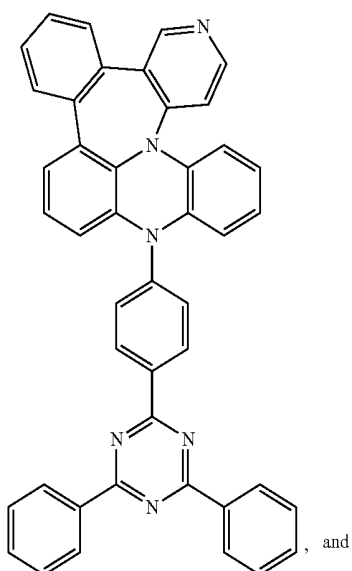
9. The fused cyclic compound according to claim 4, wherein the fused cyclic compound is an organic electroluminescent material.

10. The fused cyclic compound according to claim 5, wherein the fused cyclic compound is an organic electroluminescent material.

11. A method for preparing a fused cyclic compound according to claim 1, wherein

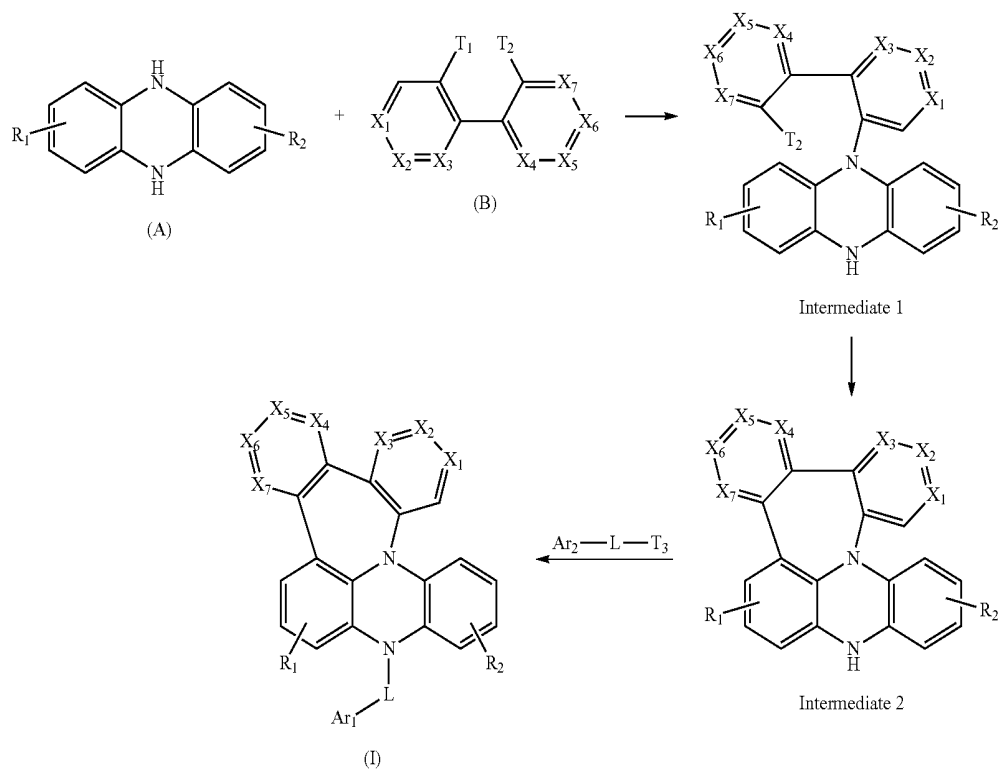
the compound of Formula (I) is synthesized through the following steps:

subjecting a compound of Formula (A) and a compound of Formula (B) as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 1; cyclizing the intermediate 1, to obtain an intermediate 2; and subjecting the intermediate 2 and a compound T_3-L-Ar_1 to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (I),



(D-20)

where the synthesis route for the compound of Formula (I) is shown below:

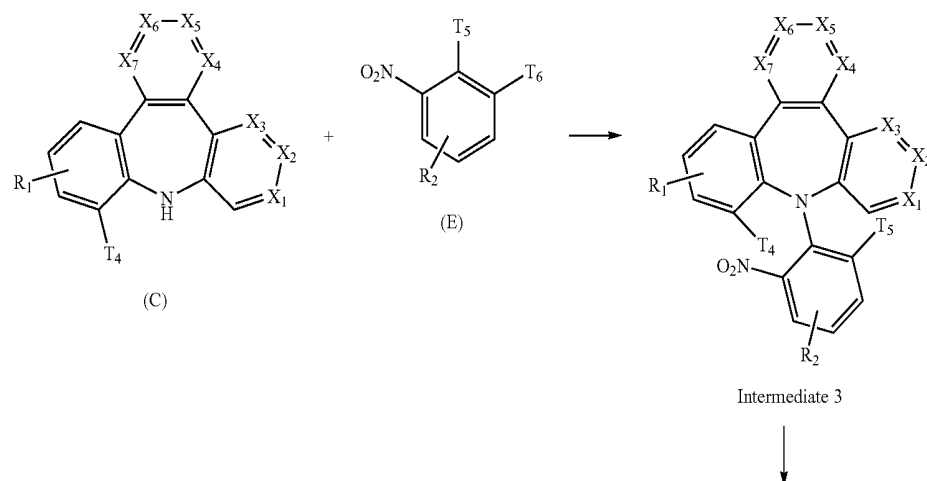


the compound of Formula (II) is synthesized through the following steps:

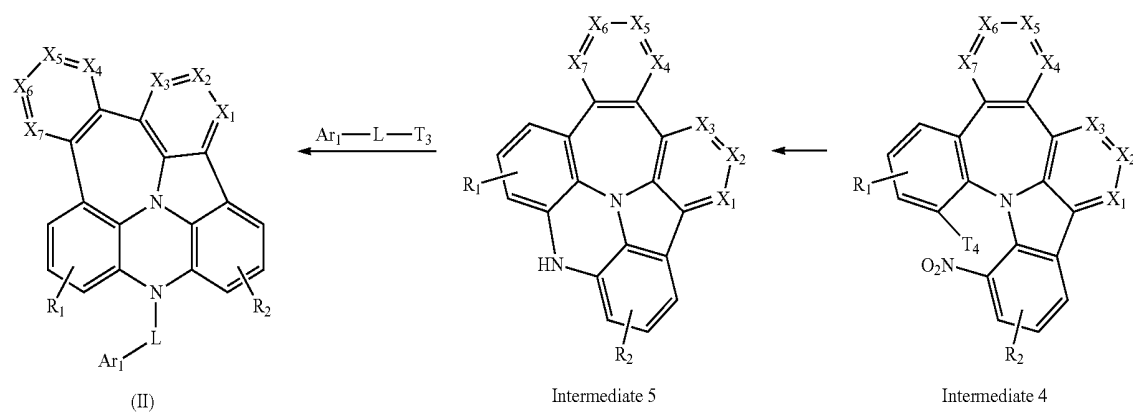
subjecting a compound of Formula (C) and a compound of Formula (E) as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 3; cyclizing the intermediate 3, to obtain an intermediate 4; reducing the nitro group of the

intermediate 4 and then subjecting the intermediate 4 to a coupling reaction, to obtain an intermediate 5; and subjecting the intermediate 5 and a compound T_3-L-Ar_1 to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (II),

where the synthesis route for the compound of Formula (II) is shown below:



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where T_1 - T_6 are each independently selected from hydrogen, fluoro, chloro, bromo or iodo.

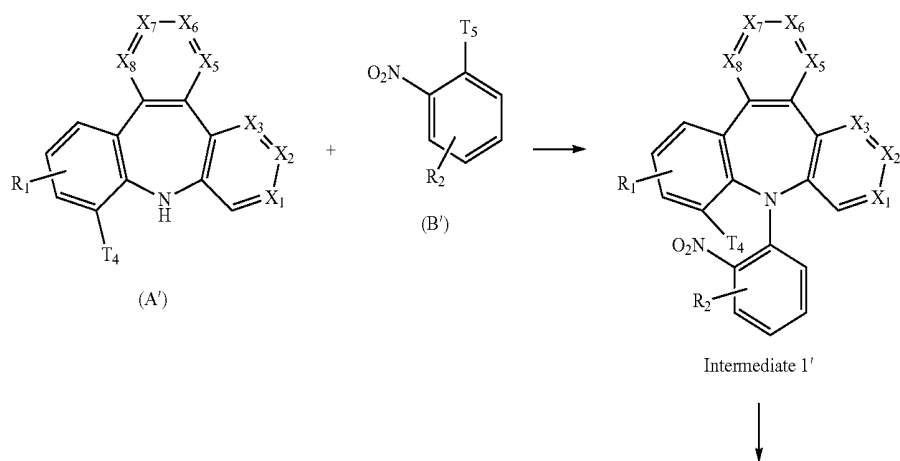
12. A method for preparing a fused cyclic compound according to claim 1, wherein

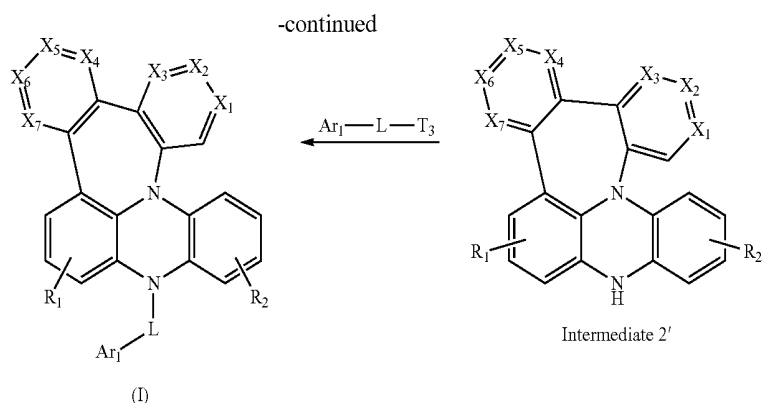
the compound of Formula (I) is synthesized through the following steps:

subjecting a compound of Formula (A') and a compound of Formula (B') as starting materials to a coupling

reaction in the presence of a catalyst, to obtain an intermediate 1'; cyclizing the intermediate 1', to obtain an intermediate 2'; and subjecting the intermediate 2' and a compound $\text{T}_3\text{---L---Ar}_1$ to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (I).

where the synthesis route for the compound of Formula (I) is shown below:





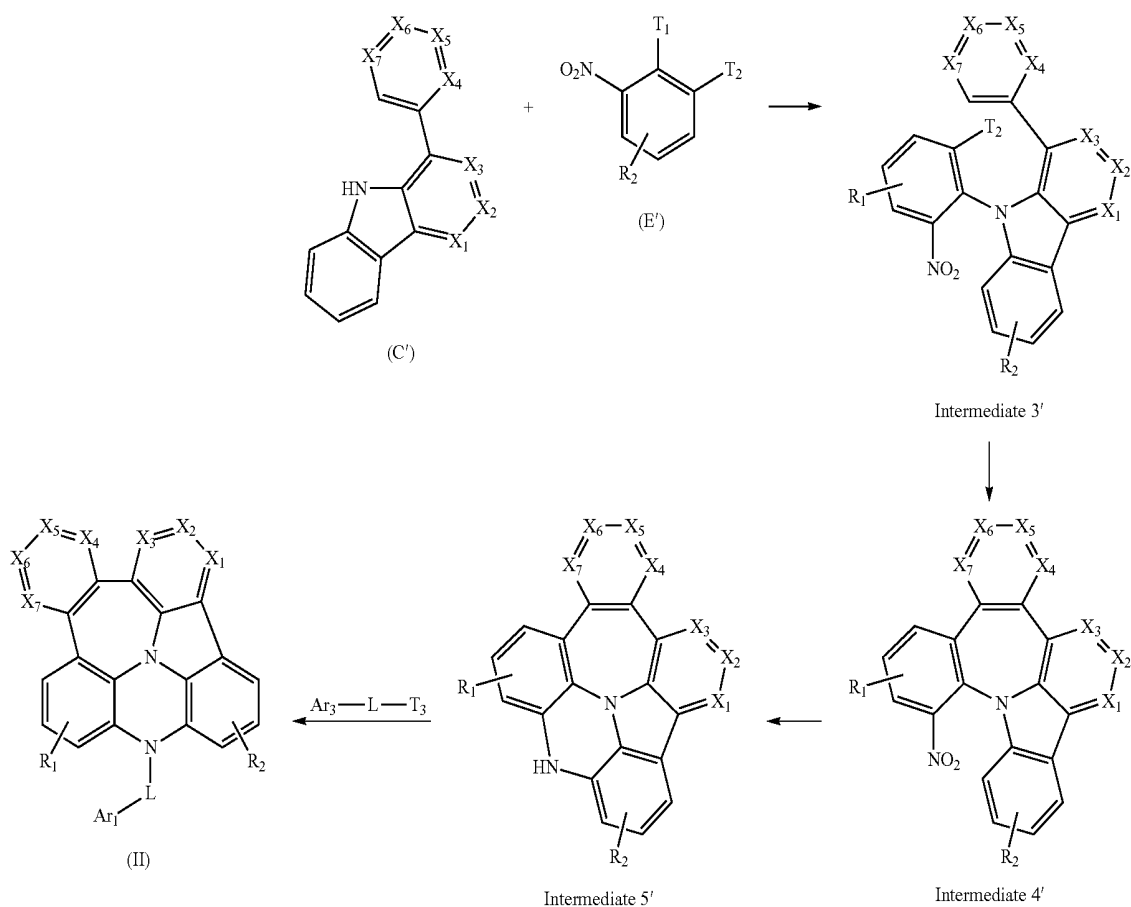
the compound of Formula (II) is synthesized through the following steps:

subjecting a compound of Formula (C') and a compound of Formula (E') as starting materials to a coupling reaction in the presence of a catalyst, to obtain an intermediate 3';

cyclizing the intermediate 3', to obtain an intermediate 4';
reducing the nitro group of the intermediate 4' and then

subjecting the intermediate 4' to a coupling reaction, to obtain an intermediate 5'; and subjecting the intermediate 5' and a compound T_3-L-Ar_1 to a substitution or coupling reaction in the presence of a catalyst, to obtain the compound of Formula (II);

where the synthesis route for the compound of Formula (II) is shown below:



where T_1 - T_5 are each independently selected from hydrogen, fluoro, chloro, bromo or iodo.

13. An organic light-emitting device, having at least one functional layer containing a fused cyclic compound according to claim 1.

14. The organic light-emitting device according to claim 13, wherein the functional layer is a light emitting layer.

15. The organic light-emitting device according to claim 14, wherein the material of the light emitting layer comprises a host material and a guest luminescent dye, where the host material is the fused cyclic compound.

* * * * *

专利名称(译)	稠环化合物及其制备方法和用途		
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摘要(译)

本发明涉及通过控制芳香族环与杂环的共轭而具有式化合物结构的稠合环状化合物。电子传输性能达到平衡，而稠合环状化合物的空穴性能得到改善。该化合物具有较高的三重态能级和玻璃化转变温度。材料分子不容易结晶。该化合物可确保将能量转移至客体材料。调节取代基可改善电子和空穴的传输性能，减少能级之间的差异，扩大载流子的重组区域，并防止三重态-三重态激子湮灭。本发明还涉及一种有机发光器件，该有机发光器件具有至少一个功能层，该功能层包含在发光层中用作主体材料的稠合环状化合物。发光层的能级变得与载流子传输层的能级匹配，从而降低了器件的驱动电压，同时提高了器件的发光效率。

