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**Hsin et al.**

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(54) **ORGANIC ELECTROLUMINESCENT COMPOUND AND ORGANIC ELECTROLUMINESCENT DEVICE CONTAINING THE SAME**

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(22) Filed: **Dec. 28, 2018**

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**Related U.S. Application Data**

(60) Continuation-in-part of application No. 16/162,833, filed on Oct. 17, 2018, which is a division of (Continued)

(51) **Int. Cl.**  
*H01L 51/00* (2006.01)  
*H01L 51/50* (2006.01)

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(52) **U.S. Cl.**  
CPC ..... *H01L 51/0067* (2013.01); *C07D 213/06* (2013.01); *C07D 401/14* (2013.01); (Continued)

(58) **Field of Classification Search**  
CPC .. *C07D 213/06*; *C07D 401/14*; *C07D 405/14*; *C07D 409/14*; *C07D 471/04*; (Continued)

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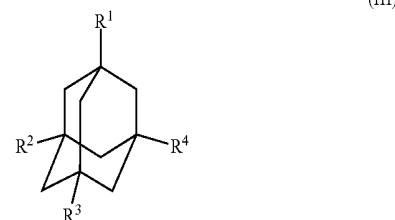
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*Primary Examiner* — Erich A Leeser

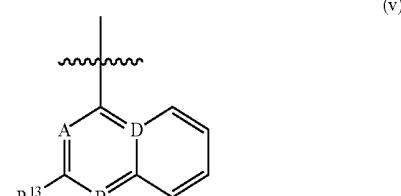
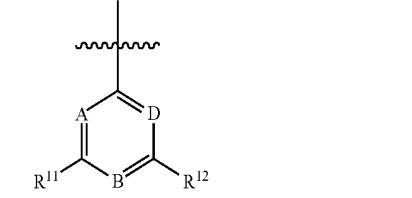
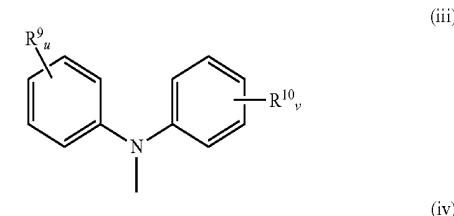
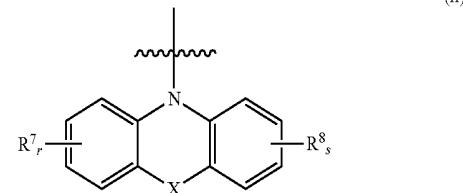
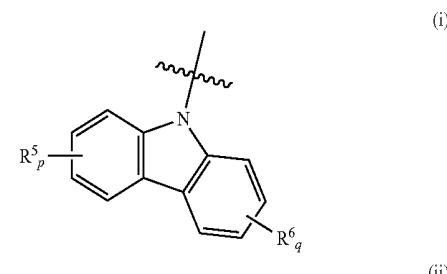
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(57) **ABSTRACT**

The present disclosure provides an organic electroluminescent compound represented by the following formula (III):

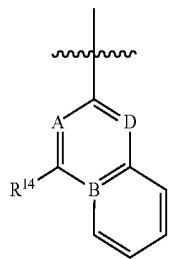


Wherein each of R<sup>1</sup> to R<sup>4</sup> is independently selected from the group consisting of hydrogen and the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii), and at least two of the R<sup>1</sup> to R<sup>4</sup> are independently selected from the group consisting of the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii):

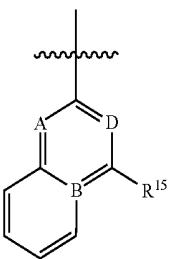


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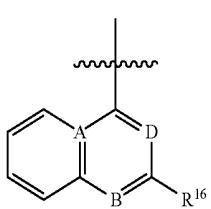
-continued



(vi)



(vii)



(viii)

**Related U.S. Application Data**

application No. 15/703,506, filed on Sep. 13, 2017,  
now Pat. No. 10,135,001.

**(51) Int. Cl.**

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**C07D 409/14** (2006.01)  
**C07D 405/14** (2006.01)  
**C07D 401/14** (2006.01)  
**C07D 213/06** (2006.01)  
**C07F 7/08** (2006.01)  
**C07F 5/02** (2006.01)  
**C09K 11/06** (2006.01)

**(52) U.S. Cl.**

CPC ..... **C07D 405/14** (2013.01); **C07D 409/14** (2013.01); **C07D 471/04** (2013.01); **C07F 5/027** (2013.01); **C07F 7/0812** (2013.01); **C09K 11/06** (2013.01); **H01L 51/005** (2013.01); **H01L 51/0052** (2013.01); **H01L 51/0054** (2013.01); **H01L 51/0055** (2013.01); **H01L 51/0058** (2013.01); **H01L 51/0065** (2013.01); **H01L 51/0068** (2013.01); **H01L 51/0072** (2013.01); **H01L 51/0094** (2013.01); **C09K 2211/1011** (2013.01); **C09K 2211/1018** (2013.01); **H01L 51/5012** (2013.01); **H01L 51/5016** (2013.01)

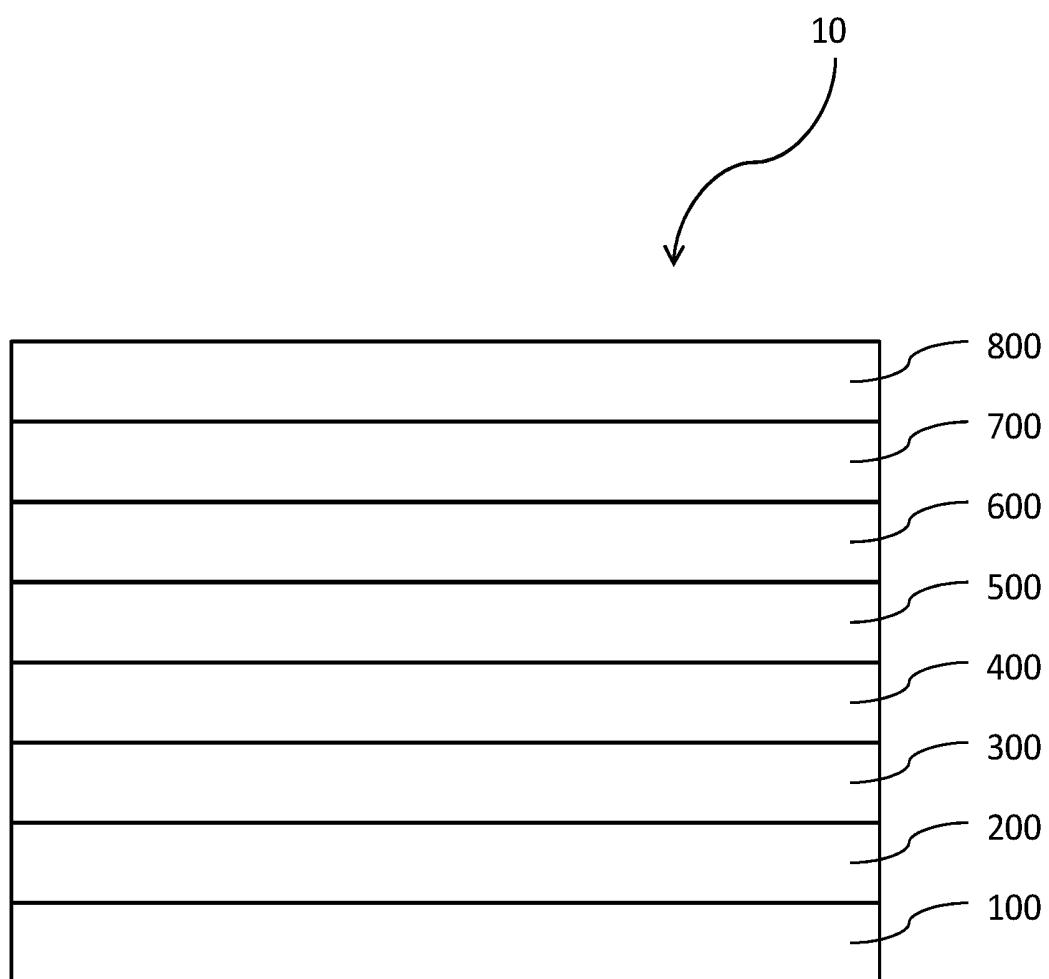
**(58) Field of Classification Search**

CPC ..... C07F 5/027; C07F 7/0812; C09K 11/06; C09K 2211/1011; C09K 2211/1018; H01L 51/005; H01L 51/0054; H01L 51/0055; H01L 51/0058; H01L 51/0065; H01L 51/0067; H01L 51/0068; H01L 51/0072; H01L 51/0094; H01L 51/5012; H01L 51/5016

See application file for complete search history.

**14 Claims, 1 Drawing Sheet**

wherein R<sup>5</sup>, R<sup>6</sup>, R<sup>7</sup>, R<sup>8</sup>, R<sup>9</sup>, R<sup>10</sup>, R<sup>11</sup>, R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup>, R<sup>16</sup>, p, q, r, s, t, u, v, A, B and D are each as defined in the description.



**ORGANIC ELECTROLUMINESCENT  
COMPOUND AND ORGANIC  
ELECTROLUMINESCENT DEVICE  
CONTAINING THE SAME**

**CROSS-REFERENCE TO RELATED  
APPLICATION**

This application is a continuation-in-part application of U.S. patent application Ser. No. 16/162,833, filed Oct. 17, 2018, which is a Divisional Application of U.S. patent application Ser. No. 15/703,506, filed Sep. 13, 2017. The entire disclosure of each of the above-described patent applications is incorporated herein by reference.

**BACKGROUND**

Due to great potential application to flexible display devices, organic light emitting diodes (OLEDs) have recently become very important to the scientific community and the display industry, and now attract much focus in research and development. An OLED is a light-emitting diode (LED) in which a film of organic compounds is placed between two conductors and emits light in response to excitation such as by an electric current. OLEDs are useful in displays such as television screens, computer monitors, mobile phones, and tablets. OLED devices are self-luminous devices, and have been actively studied for their brightness, superior visibility, and the ability to display clearer images in comparison with liquid crystal devices.

However, the OLED device technology is currently experiencing an obstacle in the development process. A main issue is that light-emitting efficiency cannot meet practical demand, so the development of the OLED technology is greatly limited. One of the factors affecting the luminous efficiency of the OLED device is the efficiency of transporting carriers, including electrons and holes.

**BRIEF DESCRIPTION OF THE DRAWINGS**

Aspects of the present disclosure are best understood from the following detailed description when read with the accompanying figures. It is emphasized that, in accordance with the standard practice in the industry, various features are not drawn to scale. In fact, the dimensions of the various features may be arbitrarily increased or reduced for clarity of discussion.

FIG. 1 is a view showing an embodiment of an organic electroluminescent device in accordance with some embodiments of the present disclosure.

**DETAILED DESCRIPTION OF THE  
DISCLOSURE**

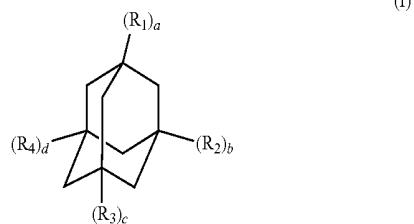
The following disclosure provides many different embodiments, or examples, for implementing different features of the provided subject matter. Specific examples of components and arrangements are described below to simplify the present disclosure. These are, of course, merely examples and are not intended to be limiting.

OLED compounds rely on the radiative decay of molecular excited states (excitors) generated by recombination of electrons and holes in a host transport material. The nature of excitation results in interactions between electrons and holes that split the excited states into bright singlets and dark triplets. Traditional phosphorescent OLEDs rely on the mixing of singlet and triplet states due to spin-orbital (SO)

interaction. This results in energy harvesting from all higher singlet and triplet states, followed by phosphorescence (relatively short-lived emission from the excited triplet). The shortened triplet lifetime reduces triplet exciton annihilation by charges and other excitons.

Therefore, there is a need for OLEDs that can reach higher excitation states without rapid degradation. It has now been discovered that thermally activated delayed fluorescence (TADF) can transfer population between singlet levels and triplet sublevels in a relevant timescale, such as, for example, 110 μs. The present disclosure provides organic electroluminescent compounds that are capable of fluorescing or phosphorescing at higher energy excitation states than the traditional organic electroluminescent compounds. The organic electroluminescent compounds of the present disclosure may improve carrier transporting ability. In some embodiments, the organic electroluminescent compounds of the present disclosure can be used in an electronic device or an optoelectronic device such as a light-emitting element, light-emitting device or lighting device.

In some embodiments, the present invention provides an organic electroluminescent compound represented by the following formula (I):



wherein

R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> each independently represents a substituted or unsubstituted (C<sub>6</sub>-C<sub>30</sub>) aryl group, a substituted or unsubstituted 3- to 30- membered heteroaryl group, —N<sub>5</sub>R<sub>6</sub>, —SiR<sub>7</sub>R<sub>8</sub>R<sub>9</sub>, —SR<sub>10</sub>, —OR<sub>11</sub>, a cyano group, a nitro group or a hydroxyl group;

R<sub>5</sub> to R<sub>11</sub> each independently represents hydrogen, deuterium, a halogen, a substituted or unsubstituted (C<sub>1</sub>-C<sub>30</sub>) alkyl group, a substituted or unsubstituted (C<sub>6</sub>-C<sub>30</sub>) aryl group or a substituted or unsubstituted 3- to 30-membered heteroaryl group; or is linked to one or more adjacent substituents to form a mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced by at least one atom selected from nitrogen, oxygen and sulfur;

a and c each independently represents an integer of 1 to 3; wherein a or c is an integer of 1 or more, and each of R<sub>1</sub> or each of R<sub>3</sub> is the same or different;

b and d each independently represents an integer of 1 to 3; wherein b or d is an integer of 1 or more, and each of R<sub>2</sub> or each of R<sub>4</sub> is the same or different; and wherein the heteroaryl group contains at least one atom selected from B, N, O, S, P(=O), Si and P.

In some embodiments of the present disclosure, substituents of the substituted groups in R<sub>1</sub> to R<sub>4</sub> and R<sub>5</sub> to R<sub>11</sub> each independently includes at least one selected from the group consisting of deuterium, a halogen, a (C<sub>1</sub>-C<sub>30</sub>)alkyl group, a (C<sub>1</sub>-C<sub>30</sub>)alkyl group substituted with a halogen, a (C<sub>6</sub>-C<sub>30</sub>)aryl group, a 3- to 30-membered heteroaryl group, a 3- to 30-membered heteroaryl group substituted with a (C<sub>6</sub>-C<sub>30</sub>)aryl group, a (C<sub>6</sub>-C<sub>30</sub>)aryl group substituted with a 3- to 30-membered heteroaryl group, a (C<sub>3</sub>-C<sub>30</sub>)cycloalkyl group, a 5- to 7-membered heterocycloalkyl group, a tri(C<sub>1</sub>-C<sub>30</sub>)silyl group, a (C<sub>1</sub>-C<sub>30</sub>)alkoxy group, a (C<sub>1</sub>-C<sub>30</sub>)alkylsulfonyl group, a (C<sub>1</sub>-C<sub>30</sub>)alkylsulfonyloxy group, a (C<sub>1</sub>-C<sub>30</sub>)alkylsulfonylalkyl 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C30)alkylsilyl group, a tri(C6-C30)arylsilyl group, a di(C1-C30)alkyl(C6-C30)arylsilyl group, a (C1-C30)alkyldi(C6-C30)arylsilyl group, a (C2-C30)alkenyl group, a (C2-C30)alkynyl group, a cyano group, a di(C1-C30)alkylamino group, a di(C6-C30)aryl amino group, a (C1-C30)alkyl(C6-C30)aryl amino group, a di(C6-C30)arylboronyl group, a di(C1-C30)alkylboronyl group, a (C1-C30)alkyl(C6-C30)arylboronyl group, a (C6-C30)aryl(C1-C30)alkyl group, a (C1-C30)alkyl(C6-C30)aryl group, a carboxyl group, a nitro group and a hydroxyl group.

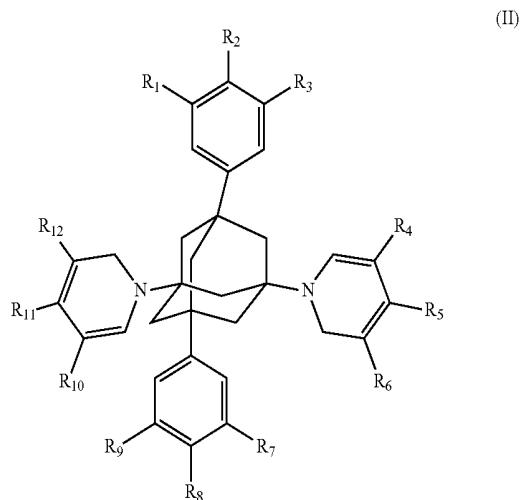
In some embodiments of the present disclosure, the terms "alkyl" and "alkoxy," and any alkyl moiety that is comprised in substituents, include both a linear structure and a branched structure; and the term "cycloalkyl" includes a mono- or polycyclic hydrocarbon or a substituted or unsubstituted (C7-C30) bicycloalkyl group. The term "aryl" refers to an organic radical derived from an aromatic hydrocarbon by removing one hydrogen atom; includes a monocyclic ring or fused ring each of whose rings has 4 to 7, preferably 5 or 6, ring backbone atoms; may be formed by linking two or more aryl groups to one another via one or more single bonds; and includes phenyl, biphenyl, terphenyl, naphthyl, anthryl, indenyl, fluorenyl, phenanthrenyl, triphenylenyl, pyrenyl, perylenyl, chrysene, naphthacene, fluoranthene, etc., wherein said naphthyl includes 1-naphthyl and 2-naphthyl, said anthryl includes 1-anthryl, 2-anthryl and 9-anthryl, and said fluorenyl includes 1-fluorenyl, 2-fluorenyl, 3-fluorenyl, 4-fluorenyl and 9-fluorenyl. The term "heteroaryl" refers to an aryl having 1 to 4 heteroatoms selected from the group consisting of B, N, O, S, P(=O), Si and P, and carbon atoms as remaining ring backbone atoms other than said heteroatom; is a monocyclic ring or fused ring condensed with at least one benzene ring; may be partially saturated; may be formed by linking at least one heteroaryl group to another heteroaryl or aryl group via one or more single bonds; may be a divalent aryl group whose ring backbone heteroatom is oxidized or quaternarized, for example, to form an N-oxide or a quaternary salt; and includes a monocyclic ring-type heteroaryl including furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, etc., a fused ring-type heteroaryl including benzofuranyl, benzothiophenyl, isobenzofuranyl, benzimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenanthridinyl, benzodioxolyl, dibenzofuranyl, dibenzothiophenyl, etc., N-oxides thereof (for example, pyridyl N-oxide, quinolyl N-oxide), and quaternary salts thereof.

In some embodiments of the present disclosure, R<sub>1</sub> to R<sub>4</sub> each independently represents hydrogen, deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, biphenyl, fluorenyl, fluoranthenyl, triphenylenyl, pyrenyl, chrysenyl, naphthacenyl, perylenyl, pyridyl, pyrrolyl, furanyl, thiophenyl, imidazolyl, benzimidazolyl, indenyl, pyrazinyl, pyrimidinyl, pyridazinyl, quinolyl, triazinyl, benzofuranyl, dibenzofuranyl, benzothiophenyl, dibenzothiophenyl, pyrazolyl, indolyl, carbazolyl, thiazolyl, oxazolyl, benzothiazolyl, benzoxazolyl, phenanthrolinyl or N-carbazolyl.

In some embodiments of the present disclosure, each of  $R_1$  to  $R_4$  and  $R_5$  to  $R_{11}$  may independently be further

substituted with at least one selected from the group consisting of deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, 5 hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, biphenyl, fluorenyl, fluoranthenyl, triphenylenyl, pyrenyl, chrysenyl, naphthacene-10 nyl, perylenyl, fluorotrimethylsilyl, triethylsilyl, tripropylsilyl, tri(t-butyl)silyl, t-butyldimethylsilyl, dimethylphenylsilyl, carbazolyl and triphenylsilyl, and more preferably at least one selected from the group consisting of deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 15 2-ethylhexyl, n-nonyl and decyl.

13 Accordingly, in one embodiment, the present invention is an organic electroluminescent compound represented by the following formula (II):



40 wherein  $R_1$  to  $R_{12}$  each independently represents hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30) alkyl group, a substituted or unsubstituted (C6-C30) aryl group or a substituted or unsubstituted 3- to 30-membered heteroaryl group; or is linked to one or more adjacent substituents to form a mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced by at least one atom selected from nitrogen, oxygen and sulfur; and the heteroaryl group contains at least one atom selected from B, N, O, S, P(=O), Si and P.

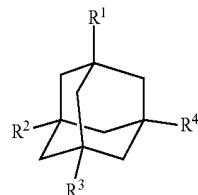
50 In some embodiments of the present disclosure, substituents of the substituted groups in  $R_1$  to  $R_{12}$  include independently at least one selected from the group consisting of deuterium, a halogen, a (C1-C30)alkyl group, a (C1-C30)alkyl group substituted with a halogen, a (C6-C30)aryl group, a 3- to 30-membered heteroaryl group, a 3- to 30-membered heteroaryl group substituted with a (C6-C30)aryl group, a (C6-C30)aryl group substituted with a 3- to 30-membered heteroaryl group, a (C3-C30)cycloalkyl group, a 5- to 7-membered heterocycloalkyl group, a tri(C1-C30)alkylsilyl group, a tri(C6-C30)arylsilyl group, a di(C1-C30)alkyl(C6-C30)arylsilyl group, a (C1-C30)alkylid(C6-C30)arylsilyl group, a (C2-C30)alkenyl group, a (C2-C30)alkynyl group, a cyano group, a di(C1-C30)alkylamino group, a di(C6-C30)arylamino group, a (C1-C30)alkyl(C6-C30)arylamino group, a di(C6-C30)arylboronyl group, a di(C1-C30)alkylboronyl group, a (C1-C30)alkyl(C6-C30)

arylboronyl group, a (C6-C30)aryl(C1-C30)alkyl group, a (C1-C30)alkyl(C6-C30)aryl group, a carboxyl group, a nitro group, and a hydroxyl group.

In some embodiments of the present disclosure, the terms “alkyl” and “alkoxy,” and any alkyl moiety which is comprised in substituents, include both a linear structure and a branched structure; and the term “cycloalkyl” includes a mono- or polycyclic hydrocarbon such as a substituted or unsubstituted (C7-C30) bicycloalkyl group. The term “aryl” refers to an organic radical derived from an aromatic hydrocarbon by removing one hydrogen atom; includes a monocyclic ring or fused ring each of whose rings has 4 to 7, preferably 5 or 6, ring backbone atoms; may be formed by linking two or more aryl groups to one another via one or more single bonds; and includes phenyl, biphenyl, terphenyl, naphthyl, anthryl, indenyl, fluorenyl, phenanthrenyl, triphenylenyl, pyrenyl, perylenyl, chryslenyl, naphthacenyl, fluoranthenyl, etc., wherein said naphthyl includes 1-naphthyl and 2-naphthyl, said anthryl includes 1-anthryl, 2-anthryl and 9-anthryl and said fluorenyl includes 1-fluorenyl, 2-fluorenyl, 3-fluorenyl, 4-fluorenyl and 9-fluorenyl. The term “heteroaryl” refers to an aryl having 1 to 4 heteroatoms selected from the group consisting of B, N, O, S, P(=O), Si and P, and carbon atoms as remaining ring backbone atoms other than said heteroatom; is a monocyclic ring or fused ring condensed with at least one benzene ring; may be partially saturated; may be one formed by linking at least one heteroaryl group to other heteroaryl or aryl group via one or more single bonds; may be a divalent aryl group whose ring backbone heteroatom is oxidized or quaternarized, for example, to form an N-oxide or a quaternary salt; and includes a monocyclic ring-type heteroaryl including furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, 35 thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, etc., a fused ring-type heteroaryl including benzofuranyl, benzothiophenyl, isobenzofuranyl, benzoimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenanthridinyl, benzodioxolyl, dibenzofuranyl, dibenzothiophenyl, etc., N-oxides thereof (for example, pyridyl N-oxide, 40 quinolyl N-oxide), and quaternary salts thereof.

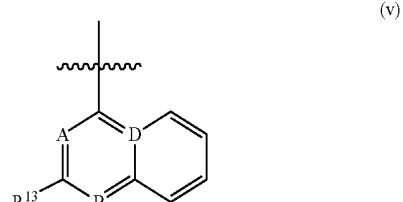
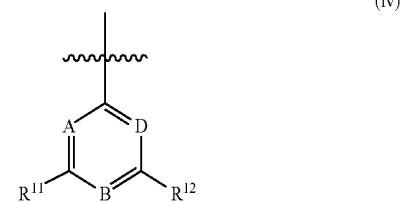
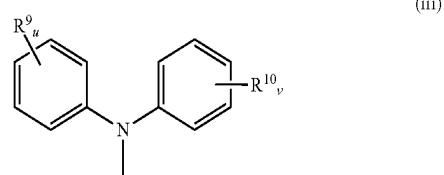
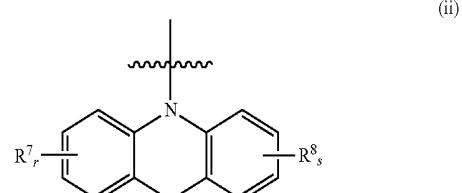
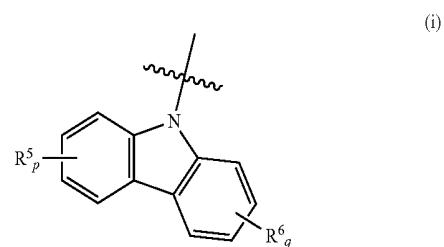
In some embodiments of the present disclosure, each of R<sub>1</sub> to R<sub>12</sub> may independently be further substituted with at least one selected from the group consisting of deuterium, 50 chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, biphenyl, fluorenyl, fluoranthenyl, 55 triphenylenyl, pyrenyl, chryslenyl, naphthacenyl, perylenyl, fluorotrimethylsilyl, triethylsilyl, tripropylsilyl, tri(t-butyl) silyl, t-butyldimethylsilyl, dimethylphenylsilyl, carbazolyl and triphenylsilyl, and more preferably at least one selected from the group consisting of deuterium, chloro, fluoro, 60 methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl and decyl.

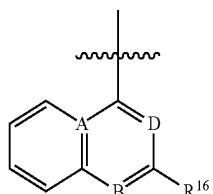
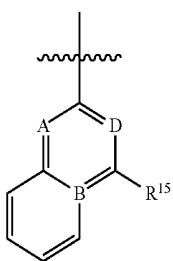
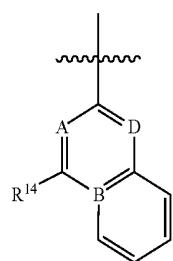
In some embodiments, the present invention provides an 65 organic electroluminescent compound represented by the following formula (III):



wherein

each of R<sup>1</sup> to R<sup>4</sup> is independently selected from the group consisting of hydrogen and the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii), and at least two of the R<sup>1</sup> to R<sup>4</sup> are independently selected from the group consisting of the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii):



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(vi)

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(vii)

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(viii)

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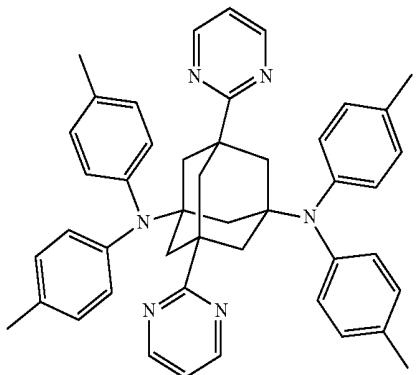
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In some embodiments, at least one of R<sup>1</sup> and R<sup>3</sup> of formula (III) is the group represented by formula (iii) and at least one of R<sup>2</sup> and R<sup>4</sup> of formula (III) is the group represented by formula (iv); and each of R<sup>9</sup> and R<sup>10</sup> is independently selected from the group consisting of hydrogen and a C<sub>1</sub>-C<sub>6</sub> alkyl group, each of u and v is independently an integer of 1, each of A and D is nitrogen, B is carbon, and each of R<sup>11</sup> and R<sup>12</sup> is independently selected from the group consisting of hydrogen and a C<sub>1</sub>-C<sub>6</sub> alkyl group.

In some embodiments, the present invention provides an organic electroluminescent compound represented by the following formula (IV):

(IV)



wherein each of R<sup>5</sup>, R<sup>6</sup>, R<sup>7</sup>, R<sup>8</sup>, R<sup>9</sup> and R<sup>10</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group; each of p, q, r, s, t, u and v is independently an integer between 1 and 4; X is selected from the group consisting of NR<sup>17</sup>, O, S, CR<sup>18</sup>, SiR<sup>19</sup>, PR<sup>20</sup> and Se; each of R<sup>17</sup>, R<sup>18</sup>, R<sup>19</sup> and R<sup>20</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group; each of A, B and, D is independently selected from the group consisting of carbon and nitrogen; and each of R<sup>11</sup>, R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup> and R<sup>16</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group.

In some embodiments, the organic electroluminescent compound represented by the following formula (III) is di-substituted. In some embodiments, the organic electroluminescent compound represented by the following formula (III) is tri-substituted. In some embodiments, the organic electroluminescent compound represented by the following formula (III) is tetra-substituted.

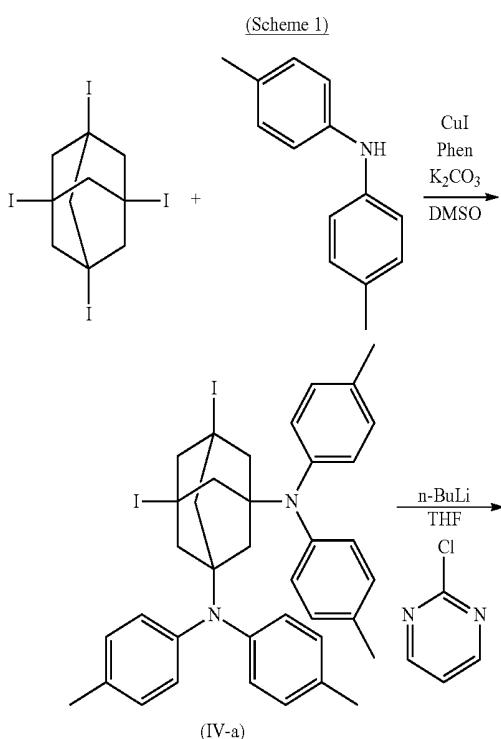
In some embodiments, at least two of R<sup>1</sup> to R<sup>4</sup> of formula (III) is independently selected from the group consisting of the groups represented by formula (iii) and formula (iv).

In some embodiments, each of R<sup>5</sup>, R<sup>6</sup>, R<sup>7</sup>, R<sup>8</sup>, R<sup>9</sup>, R<sup>10</sup>, R<sup>11</sup>, R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup> and R<sup>16</sup> is independently selected from the group consisting of hydrogen and a C<sub>1</sub>-C<sub>6</sub> alkyl group.

In some embodiments, each of A and D is nitrogen, and B is carbon.

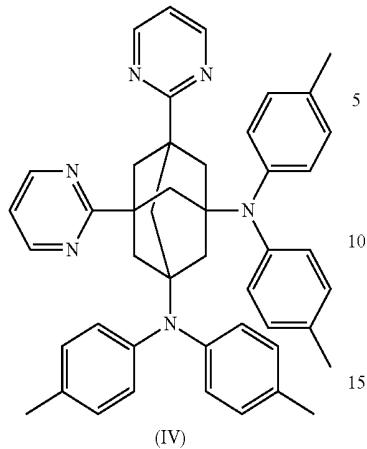
In some embodiments, at least one of R<sup>1</sup> and R<sup>3</sup> of formula (III) is the group represented by formula (iii) and at least one of R<sup>2</sup> and R<sup>4</sup> of formula (III) is the group represented by formula (iv).

In some embodiments, the present invention provides a method of preparing the organic electroluminescent compound represented by the formula (IV). In some embodiments, the organic electroluminescent compound represented by formula (IV) can be synthesized according to Scheme 1:



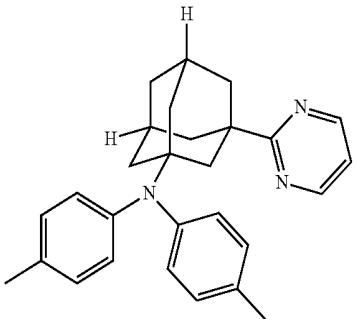
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(V)



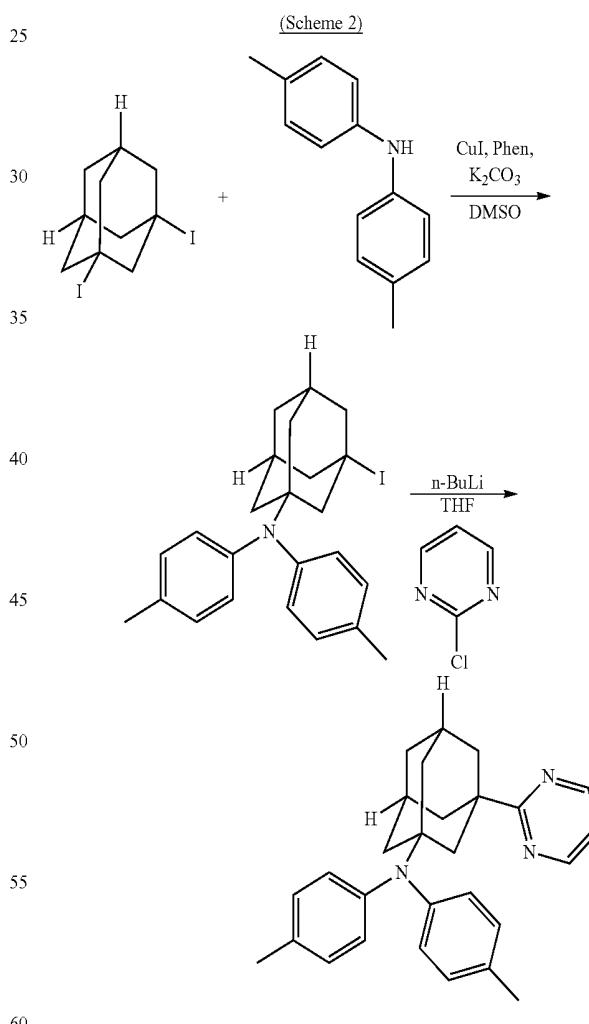
In Scheme 1, the organic electroluminescent compound represented by formula (IV) is synthesized by two steps, the first step and the second step.

In the first step, the compound represented by formula (IV-a) is synthesized as follows. 1,3,5,7-tetraiodoadamantane (1 mmol), ditolylamine (2 mmol), copper iodide (0.1 mmol), 1,10-phenanthroline (0.1 mmol), and potassium carbonate (2.5 mmol) were added into a flask under an inert gas atmosphere. DMSO (5 mL) was further added to the flask under inert gas atmosphere and the flask was heated to 120° C. for 24 hours to obtain a reaction mixture. The reaction mixture was filtered to obtain a solution. The organic solvent of the solution was washed with brine two times. The combined organic layer was dried with  $\text{Na}_2\text{SO}_4$  and the organic solvent was removed to obtain a residue. The residue was purified by silica gel chromatography to obtain the organic electroluminescent compound represented by formula (IV-a).

In the second step, the organic electroluminescent compound represented by formula (IV) is synthesized as follows. The compound represented by formula (IV-a) (0.5 mmol) and THF (10 mL) were added into a round-bottom bottle under nitrogen atmosphere. The round-bottom bottle was cooled to -78° C. by acetone- $\text{N}_2$ .  $n\text{-BuLi}$  (1.1 mmol) was further slowly added to the round-bottom bottle via syringe and stirred for 30 min at -78° C. 2-chloropyrimidine (1.1 mmol) was further added to the round-bottom bottle and stirred for 30 min at -78° C. to form a reaction mixture. The reaction mixture was warmed to room temperature, then quenched by brine and extracted with EA. The organic layer of the mixture was dried over  $\text{Na}_2\text{SO}_4$  to provide an extract. The solvent of the extract was evaporated, and the remaining residue was purified by silica gel chromatography to obtain the organic electroluminescent compound represented by formula (IV).

In some embodiments, the present invention provides an organic electroluminescent compound represented by the following formula (V):

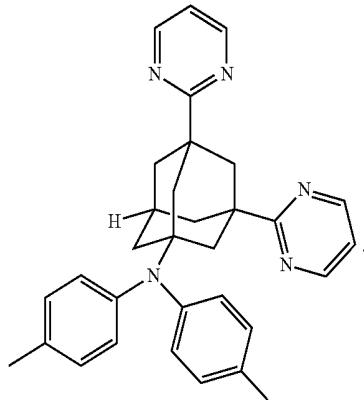
In some embodiments, the present invention provides a method of preparing the organic electroluminescent compound represented by the formula (V). In some embodiments, the organic electroluminescent compound represented by formula (IV) can be synthesized according to Scheme 2:



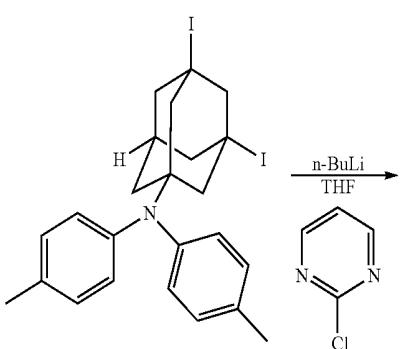
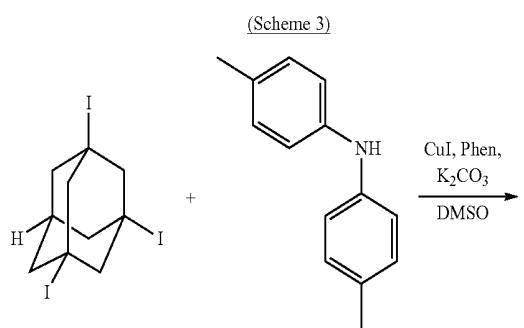
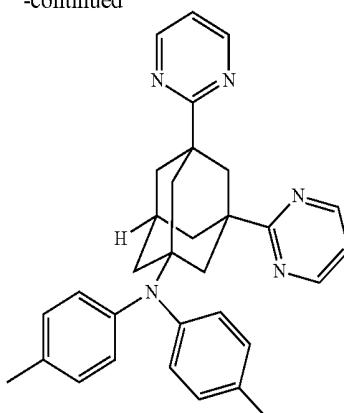
In Scheme 2, synthesis of the organic electroluminescent compound represented by formula (V) is similar to the synthesis of the organic electroluminescent compound represented by formula (IV), except that the 1,3-diiodoadamantane is used as a starting material, and the equivalent ratio of ditolylamine to 2-chloropyrimidine is 1.0 to 1.1.

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In some embodiments, the present invention provides an organic electroluminescent compound represented by the following formula (VI):

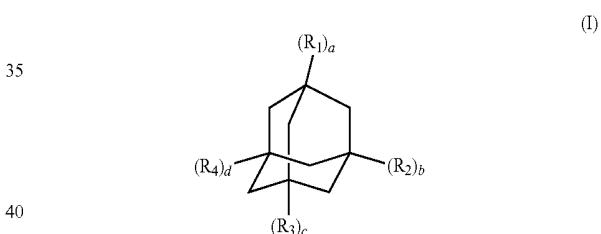


In some embodiments, the present invention provides a method of preparing the organic electroluminescent compound represented by the formula (VI). In some embodiments, the organic electroluminescent compound represented by formula (IV) can be synthesized according to Scheme 3:

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-continued

In Scheme 3, synthesis of the organic electroluminescent compound represented by formula (VI) is similar to the synthesis of the organic electroluminescent compound represented by formula (IV), except that the 1, 3, 5-triiodoadamantane is used as a starting material, and the equivalent ratio of ditolylamine to 2-chloropyrimidine is 1.0 to 2.2.

In some embodiments of the present disclosure, an organic electroluminescent device comprises: an anode, a cathode, and at least an emitting layer and an electron-transporting layer provided between the anode and the cathode; the emitting layer containing a host material which is the organic electroluminescent compound represented by the following formula (I):



wherein

$R_1$ ,  $R_2$ ,  $R_3$  and  $R_4$  each independently represents a substituted or unsubstituted (C6-C30) aryl group, a substituted or unsubstituted 3- to 30-membered heteroaryl group,  $-NR_5R_6$ ,  $-SiR_7R_8R_9$ ,  $-SR_{10}$ ,  $-OR_{11}$  a cyano group, a nitro group, or a hydroxyl group;

$R_5$  to  $R_{11}$  each independently represents hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30) alkyl group, a substituted or unsubstituted (C6-C30) aryl group, or a substituted or unsubstituted 3- to 30-membered heteroaryl group; or is linked to one or more adjacent substituents to form a mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced by at least one atom selected from nitrogen, oxygen and sulfur;

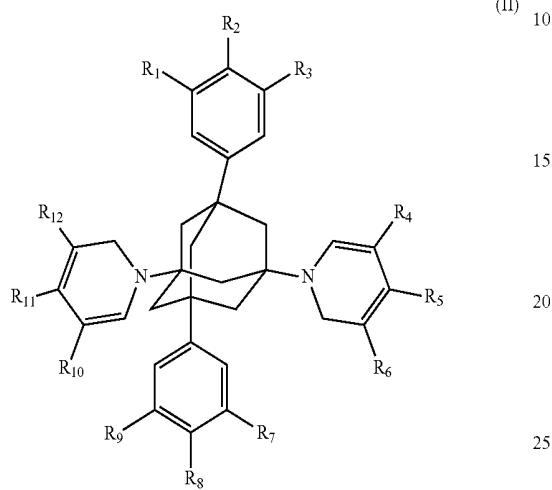
$a$  and  $c$  each independently represents an integer of 1 to 3; wherein  $a$  or  $c$  is an integer of 1 or more, and each of  $R_1$  or each of  $R_3$  is the same or different;

$b$  and  $d$  each independently represents an integer of 1 to 3; wherein  $b$  or  $d$  is an integer of 1 or more, each of  $R_2$  or each of  $R_4$  is the same or different; and wherein the heteroaryl group contains at least one atom selected from B, N, O, S, P(=O), Si and P.

In some embodiments of the present disclosure, an organic electroluminescent device comprises: an anode, a cathode, and at least an emitting layer and an electron-

transporting layer provided between the anode and the cathode; the emitting layer containing a host material which is the organic electroluminescent compound represented by the following formula (II):

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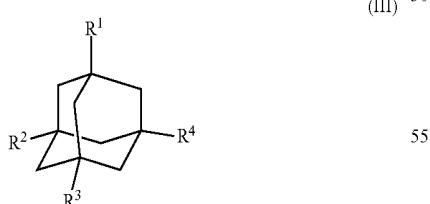


wherein R<sub>1</sub> to R<sub>12</sub> each independently represents hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30) alkyl group, a substituted or unsubstituted (C6-C30) aryl group, or a substituted or unsubstituted 3- to 30-membered heteroaryl group; or is linked to one or more adjacent substituents to form a mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced by at least one atom selected from nitrogen, oxygen and sulfur.

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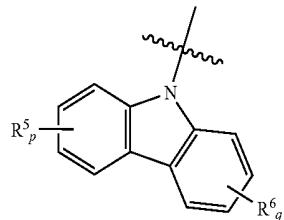
In some embodiments of the present disclosure, an organic electroluminescent device comprises: an anode, a cathode, and at least an emitting layer and an electron-transporting layer provided between the anode and the cathode; wherein the emitting layer contains a host material which is the organic electroluminescent compound represented by the following formula (III):

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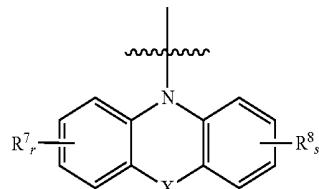


wherein each of R<sup>1</sup> to R<sup>4</sup> is independently selected from the group consisting of hydrogen and the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii), and at least two of the R<sup>1</sup> to R<sup>4</sup> are independently selected from the group consisting of the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii):

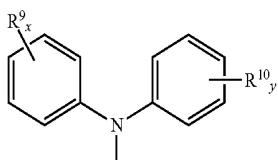
(i)



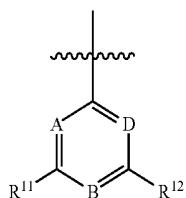
(ii)



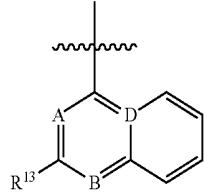
(iii)



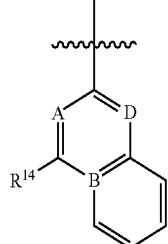
(iv)



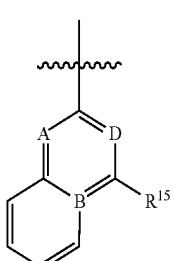
(v)



(vi)

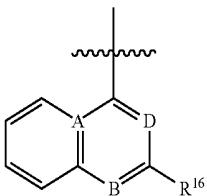


(vii)



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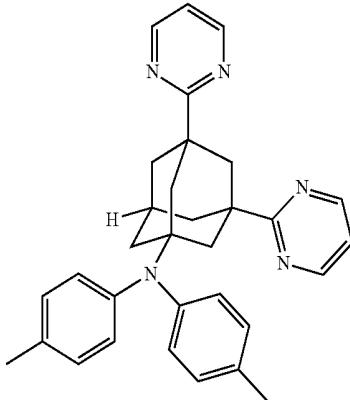
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(viii)

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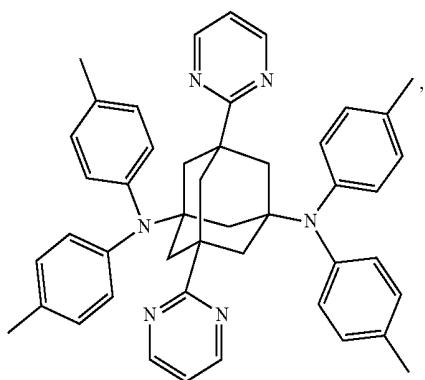


(VI)

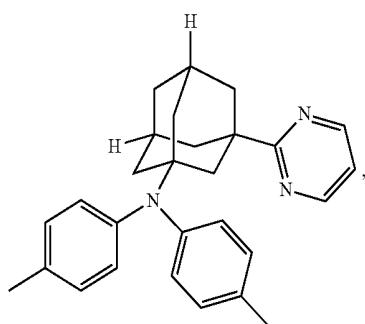
wherein each of R<sup>5</sup>, R<sup>6</sup>, R<sup>7</sup>, R<sup>8</sup>, R<sup>9</sup> and R<sup>10</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group; each of p, q, r, s, t, u and v is independently an integer between 1 and 4; X is selected from the group consisting of NR<sup>17</sup>, O, S, CR<sup>18</sup>, SiR<sup>19</sup>, PR<sup>20</sup> and Se; each of R<sup>17</sup>, R<sup>18</sup>, R<sup>19</sup> and R<sup>20</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group; each of A, B and D is independently selected from the group consisting of carbon and nitrogen; and each of R<sup>11</sup>, R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup> and R<sup>16</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group.

In some embodiments of the present disclosure, an organic electroluminescent device comprises: an anode, a cathode, and at least an emitting layer and an electron-transporting layer provided between the anode and the cathode; wherein the emitting layer contains a host material which is the organic electroluminescent compound represented by the following formula (IV), (V) or (VI):

(IV)



(V)



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In some embodiments of the present disclosure, in an organic electroluminescent (EL) device comprising at least the emitting layer and an electron-transporting layer provided between a cathode and an anode, an emitting layer contains a host material which includes the organic electroluminescent compounds represented by the above-described formula (I), (II), (III), (IV), (V) or (VI).

FIG. 1 illustrates an example of the organic EL device according to some embodiments of the present invention. An organic EL device 10 has a configuration in which an anode 200, a hole-injecting layer 300, a hole-transporting layer 400, an emitting layer 500, an electron-transporting layer 600, an electron-injecting layer 700, and a cathode 800 are stacked on a substrate 100 in an order. In some embodiments, the emitting layer 500 contains a host material of the organic electroluminescent compound represented by the above-described formula (I). In some embodiments, the emitting layer 500 contains a host material of the organic electroluminescent compound represented by the above-described formula (II). In some embodiments, the emitting layer 500 contains a host material of the organic electroluminescent compound represented by the above-described formula (III). In some embodiments, the emitting layer 500 contains a host material of the organic electroluminescent compound represented by the above-described formula (IV). In some embodiments, the emitting layer 500 contains a host material of the organic electroluminescent compound represented by the above-described formula (V). In some embodiments, the emitting layer 500 contains a host material of the organic electroluminescent compound represented by the above-described formula (VI).

In some embodiments of the present disclosure, the organic EL device is an under surface emission type or bottom emission type where light is out through a substrate. In some embodiments, the organic EL device of the present disclosure is formed on a transparent substrate. In some embodiments, the transparent substrate is a substrate for supporting the organic EL device, and is preferably a flat and smooth substrate having a light ray transmittance of 50% or more. In some embodiments, the organic EL device is an upper surface emission type or top emission type where light is out from the upper part of the device, and a light-reflecting metal such as aluminum is provided on the above substrate.

In some embodiments of the present disclosure, in the organic electroluminescent device, a mixed region of an electron transport compound and a reductive dopant, or a mixed region of a hole transport compound and an oxidative dopant, may be placed on at least one surface of a pair of electrodes. In some embodiments, the electron transport

compound is reduced to an anion, thus facilitating injection and transport of electrons from the mixed region to the electroluminescent medium. In some embodiments, the hole transport compound is oxidized to a cation, thus facilitating injection and transport of holes from the mixed region to the electroluminescent medium. In some embodiments, the oxidative dopant includes various Lewis acids and acceptor compounds, wherein the reductive dopant includes alkali metals, alkali metal compounds, alkaline earth metals, rare-earth metals, or mixtures thereof. In some embodiments, a 10 reductive dopant layer may be employed as a charge-generating layer to prepare an electroluminescent device having two or more electroluminescent layers and emitting a white light.

In some embodiments of the present disclosure, the 15 organic EL device comprises a first electrode, a second electrode and at least one organic layer between the first electrode and the second electrode. In some embodiments, the organic layer comprises a light-emitting layer. In some embodiments, the light-emitting layer comprises a composition for the organic electroluminescent device of the present disclosure and a phosphorous dopant. In some embodiments, the composition for the organic electroluminescent device comprises a host material.

In some embodiments of the present disclosure, the 20 organic EL device may further comprise at least one compound selected from the group consisting of arylamine-based compounds and styrylarylamine-based compounds in the organic layer.

In some embodiments of the present disclosure, in the 25 organic EL device, the organic layer may further comprise the organic electroluminescent compounds represented by the formulas (I), (II), (III), (IV), (V) and (VI), at least one metal selected from the group consisting of metals of Group 1, metals of Group 2, transition metals of the 4th period, 30 transition metals of the 5th period, lanthanides and organic metals of d-transition elements of the Periodic Table, or at least one complex compound comprising the metals. In some embodiments, the organic layer may further comprise a light-emitting layer and a charge-generating layer.

In some embodiments of the present disclosure, the 35 organic EL device may emit a white light by further comprising at least one light-emitting layer which comprises a blue electroluminescent compound, a red electroluminescent compound or a green electroluminescent compound, in addition to the compound of the present disclosure. In some 40 embodiments, the organic EL device may further comprise a yellow light-emitting layer or an orange light-emitting layer.

In some embodiments of the present disclosure, in the 45 organic EL device, at least one layer (referred to as "a surface layer") selected from a chalcogenide layer, a metal-halide layer and a metal-oxide layer may be placed on one or more inner surfaces of one or both electrodes. In some 50 embodiments, it is preferred that the chalcogenide (including oxides) layer of silicon or aluminum is placed on an anode surface of an electroluminescent medium layer, and the metal-halide layer or metal-oxide layer is placed on a cathode surface of an electroluminescent medium layer. Such a surface layer provides operational stability for the 55 organic electroluminescent device. Preferably, said chalcogenide includes  $\text{SiO}_x$  ( $1 \leq X \leq 2$ ),  $\text{AlO}_x$  ( $1 \leq X \leq 1.5$ ),  $\text{SiON}$ ,  $\text{SiAlON}$ , etc.; said metal halide includes  $\text{LiF}$ ,  $\text{MgF}_2$ ,  $\text{CaF}_2$ , a rare earth metal fluoride, etc.; and said metal oxide includes  $\text{Cs}_2\text{O}$ ,  $\text{Li}_2\text{O}$ ,  $\text{MgO}$ ,  $\text{SrO}$ ,  $\text{BaO}$ ,  $\text{CaO}$ , etc.

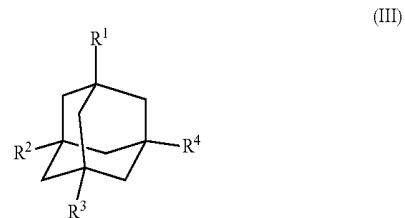
In some embodiments of the present disclosure, the use of 60 an organic electroluminescent compound represented by the

formula (I), (II), (III), (IV), (V) or (VI) as a host material in an organic EL device can provide an organic EL device with a practical efficiency and lifetime.

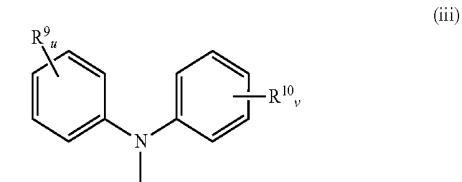
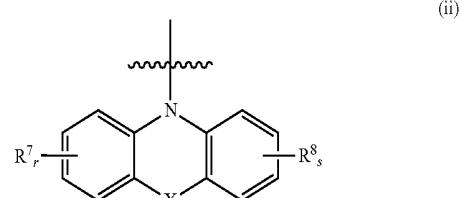
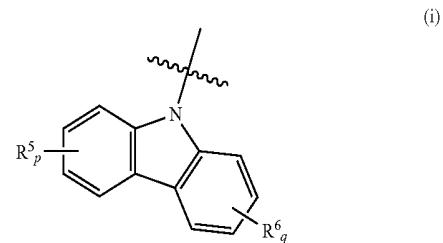
The foregoing outlines features of several embodiments 5 so that those skilled in the art may better understand the aspects of the present disclosure. Those skilled in the art should appreciate that they may readily use the present disclosure as a basis for designing or modifying other processes and structures for carrying out the same purposes and/or achieving the same advantages of the embodiments introduced herein. Those skilled in the art should also realize that such equivalent constructions do not depart from the spirit and scope of the present disclosure, and that they may make various changes, substitutions, and alterations herein without departing from the spirit and scope of the present disclosure.

What is claimed is:

1. An organic electroluminescent compound represented 20 by the following formula (III):

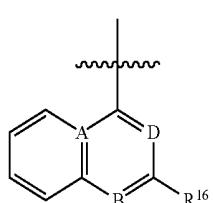
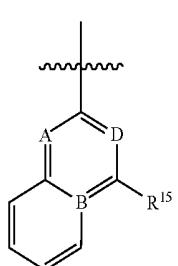
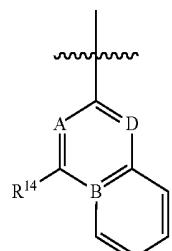
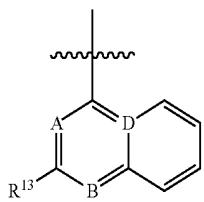
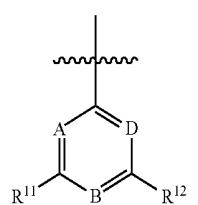


wherein each of R¹ to R⁴ is independently selected from the group consisting of hydrogen and the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii), and at least two of the R¹ to R⁴ are independently selected from the group consisting of the groups represented by formula (i), formula (ii), formula (iii), formula (iv), formula (v), formula (vi), formula (vii) and formula (viii):



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wherein each of R<sup>5</sup>, R<sup>6</sup>, R<sup>7</sup>, R<sup>8</sup>, R<sup>9</sup> and R<sup>10</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group; each of p, q, r, s, t, u and v is independently an integer between 1 and 4; X is selected from the group consisting of NR<sup>17</sup>, O, S, CR<sup>18</sup><sub>2</sub>, SiR<sup>19</sup><sub>2</sub>, PR<sup>20</sup> and Se; each of R<sup>17</sup>, and R<sup>18</sup>, R<sup>19</sup> and R<sup>20</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group; each of A and D is nitrogen, and B is carbon; and each of R<sup>11</sup>, R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup> and R<sup>16</sup> is independently selected from the group consisting of hydrogen, an aryl group, a heteroaryl group, a C<sub>1</sub>-C<sub>6</sub> alkyl group, a C<sub>1</sub>-C<sub>6</sub> alkenyl group and a C<sub>1</sub>-C<sub>6</sub> alkynyl group.

2. The organic electroluminescent compound of claim 1, wherein at least two of R<sup>1</sup> to R<sup>4</sup> is independently selected from the group consisting of the groups represented by formula (iii) and formula (iv).

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3. The organic electroluminescent compound of claim 1, wherein each of R<sup>5</sup>, R<sup>6</sup>, R<sup>7</sup>, R<sup>8</sup>, R<sup>9</sup>, R<sup>10</sup>, R<sup>11</sup>, R<sup>12</sup>, R<sup>13</sup>, R<sup>14</sup>, R<sup>15</sup> and R<sup>16</sup> is independently selected from the group consisting of hydrogen and a C<sub>1</sub>-C<sub>6</sub> alkyl group.

5 4. The organic electroluminescent compound of claim 1, wherein the organic electroluminescent compound represented by the following formula (III) is di-substituted.

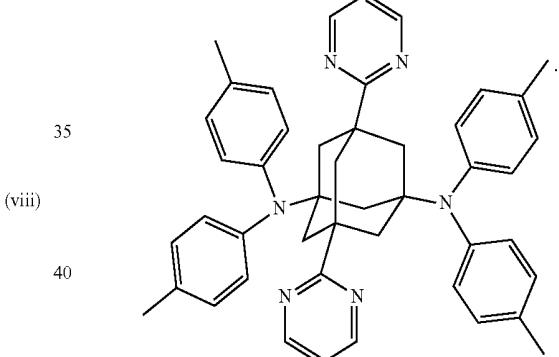
5 10 5. The organic electroluminescent compound of claim 1, wherein at least one of R<sup>1</sup> and R<sup>3</sup> is the group represented by formula (iii) and at least one of R<sup>2</sup> and R<sup>4</sup> is the group represented by formula (iv).

15 5. The organic electroluminescent compound of claim 1, wherein at least one of R<sup>1</sup> and R<sup>3</sup> is the group represented by formula (iii) and at least one of R<sup>2</sup> and R<sup>4</sup> is the group represented by formula (iv); and each of R<sup>9</sup> and R<sup>10</sup> is independently selected from the group consisting of hydrogen and a C<sub>1</sub>-C<sub>6</sub> alkyl group, each of u and v is independently an integer of 1, each of A and D is nitrogen, B is carbon, and each of R<sup>11</sup> and R<sup>12</sup> is independently selected from the group consisting of hydrogen and a C<sub>1</sub>-C<sub>6</sub> alkyl group.

20 7. The organic electroluminescent compound of claim 1, 25 wherein the organic electroluminescent compound is represented by the following formula (IV):

(vii)

30 (IV)



(viii)

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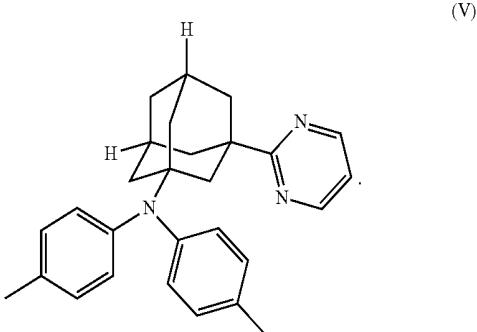
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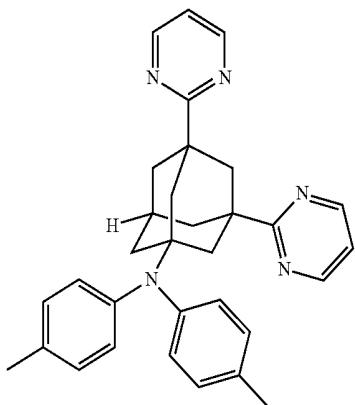
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8. The organic electroluminescent compound of claim 1, wherein the organic electroluminescent compound is represented by the following formula (V):



9. The organic electroluminescent compound of claim 1, wherein the organic electroluminescent compound is represented by the following formula (VI):

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(VI)

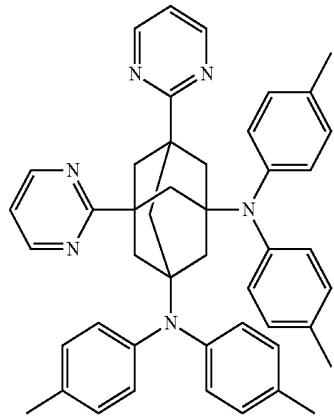
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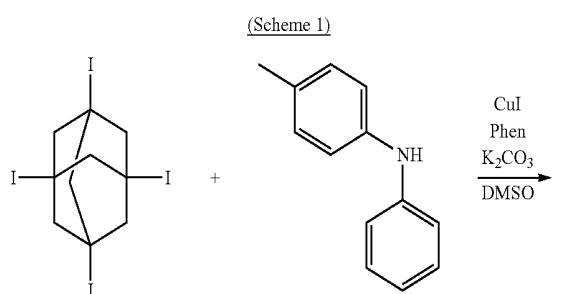
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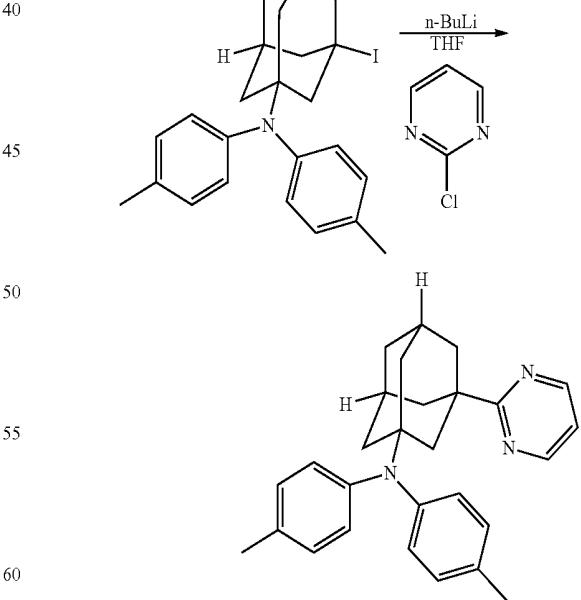
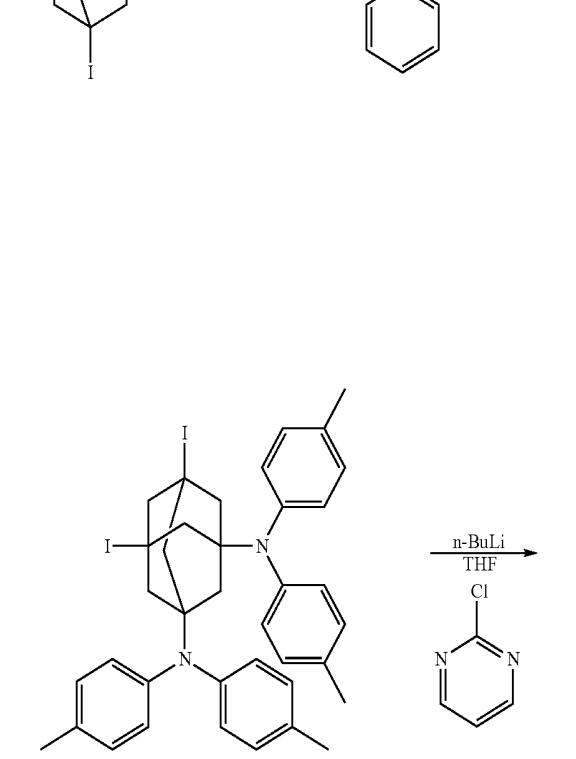
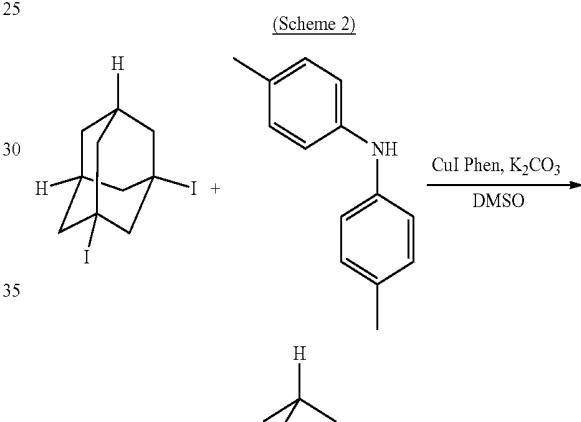
10. The organic electroluminescent compound of claim 1, wherein the organic electroluminescent compound represented by the following formula (III) is tri-substituted.

11. The organic electroluminescent compound of claim 1, wherein the organic electroluminescent compound represented by the following formula (III) is tetra-substituted.

12. The organic electroluminescent compound of claim 7, wherein the organic electroluminescent compound is represented by the following formula (IV) is synthesized according to Scheme 1:



13. The organic electroluminescent compound of claim 8, wherein the organic electroluminescent compound is represented by the following formula (V) is synthesized according to Scheme 2:

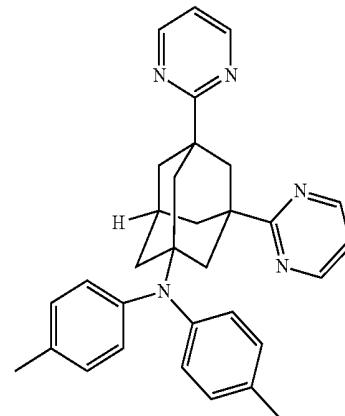
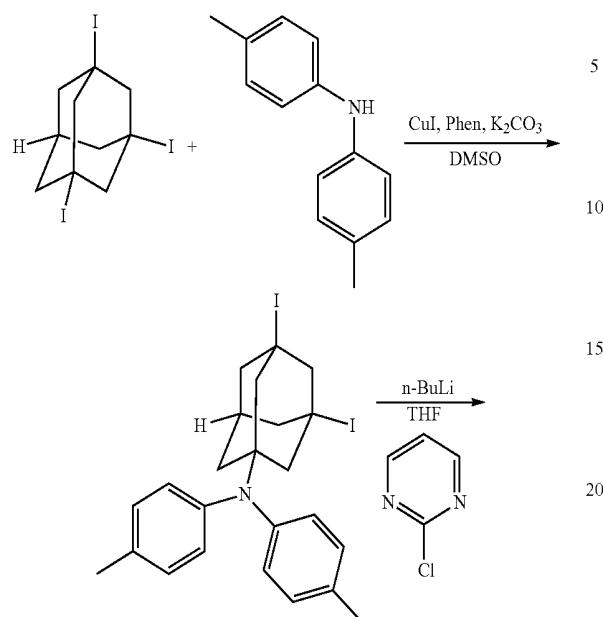


14. The organic electroluminescent compound of claim 9, wherein the organic electroluminescent compound is represented by the following formula (V) is synthesized according to Scheme 3:

**23****24**

-continued

(Scheme 3)



\* \* \* \* \*

专利名称(译)	有机电致发光化合物和包含该化合物的有机电致发光器件		
公开(公告)号	<a href="#">US10651393</a>	公开(公告)日	2020-05-12
申请号	US16/236075	申请日	2018-12-28
申请(专利权)人(译)	国际科技股份有限公司		
当前申请(专利权)人(译)	国际科技股份有限公司		
[标]发明人	HSIN MENG HUNG CHEN MIN HSIEN		
发明人	HSIN, MENG-HUNG CHEN, MIN-HSIEN		
IPC分类号	H01L51/00 C09K11/06 C07F5/02 C07F7/08 C07D401/14 C07D213/06 C07D405/14 C07D409/14 C07D471/04 H01L51/50		
CPC分类号	H01L51/0094 H01L51/0067 C07F7/0812 H01L51/0055 C07D401/14 C07F5/027 C07D213/06 H01L51 /005 C07D471/04 H01L51/0052 C09K11/06 H01L51/0054 C07D405/14 H01L51/0068 H01L51/0058 C07D409/14 H01L51/0072 H01L51/0065 C09K2211/1011 C09K2211/1018 H01L51/5016 H01L51/5012		
代理人(译)	KING , ANTHONY		
优先权	15/703506 2018-11-20 US		
其他公开文献	US20190140188A1		
外部链接	<a href="#">Espacenet</a>		

## 摘要(译)

(III)

本公开提供了一种由下式 ( III ) 表示的有机电致发光化合物：其中每个 R 1 至 R 4 独立地选自氢和由式 ( i ) , 式 ( ii ) , 式 ( iii ) , 式 ( iv ) 表示的基团，式 ( v ) , 式 ( vi ) , 式 ( vii ) 和式 ( viii ) 以及 R 1 至 R 4 中的至少两个独立地选自由式 ( i ) , 式 ( ii ) , 式 ( iii ) , 式 ( iv ) , 式 ( v ) , 式 ( vi ) , 式 ( vii ) 和式 ( viii ) 表示的基团组成的基团：其中 R 5 , R 6 , R 7 , R 8 , R 9 , R 10 , R 11 , R 12 , R 13 , R 14 , R 15 , R 16 , p , q , r , s , t , u , v , A , B 和 D 均如描述中所定义。

