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(54) **ELECTRON TRANSPORTING COMPOUNDS**

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**H01L 51/54** (2006.01)

(52) **U.S. Cl.** ..... **428/690**; 428/917; 313/504; 313/505;  
313/506; 548/440; 546/79; 546/81

(58) **Field of Classification Search** ..... 428/690,  
428/917; 313/504, 505, 506; 548/440; 546/79,  
546/81

See application file for complete search history.

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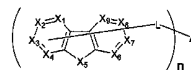
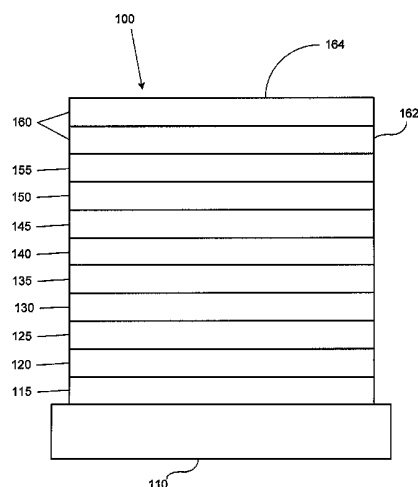
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(57) **ABSTRACT**

Compounds comprising an aza-dibenzo moiety and a con-  
densed aromatic moiety having at least three benzene rings  
are provided. In particular, the compounds may comprise an  
azadibenzofuran, azadibenzothiophene, or azadibenzosele-  
nophene joined directly or indirectly to an anthracene. The  
compounds may be used in the electron transport layer of  
organic light emitting devices to provide devices with  
improved properties.

**29 Claims, 3 Drawing Sheets**



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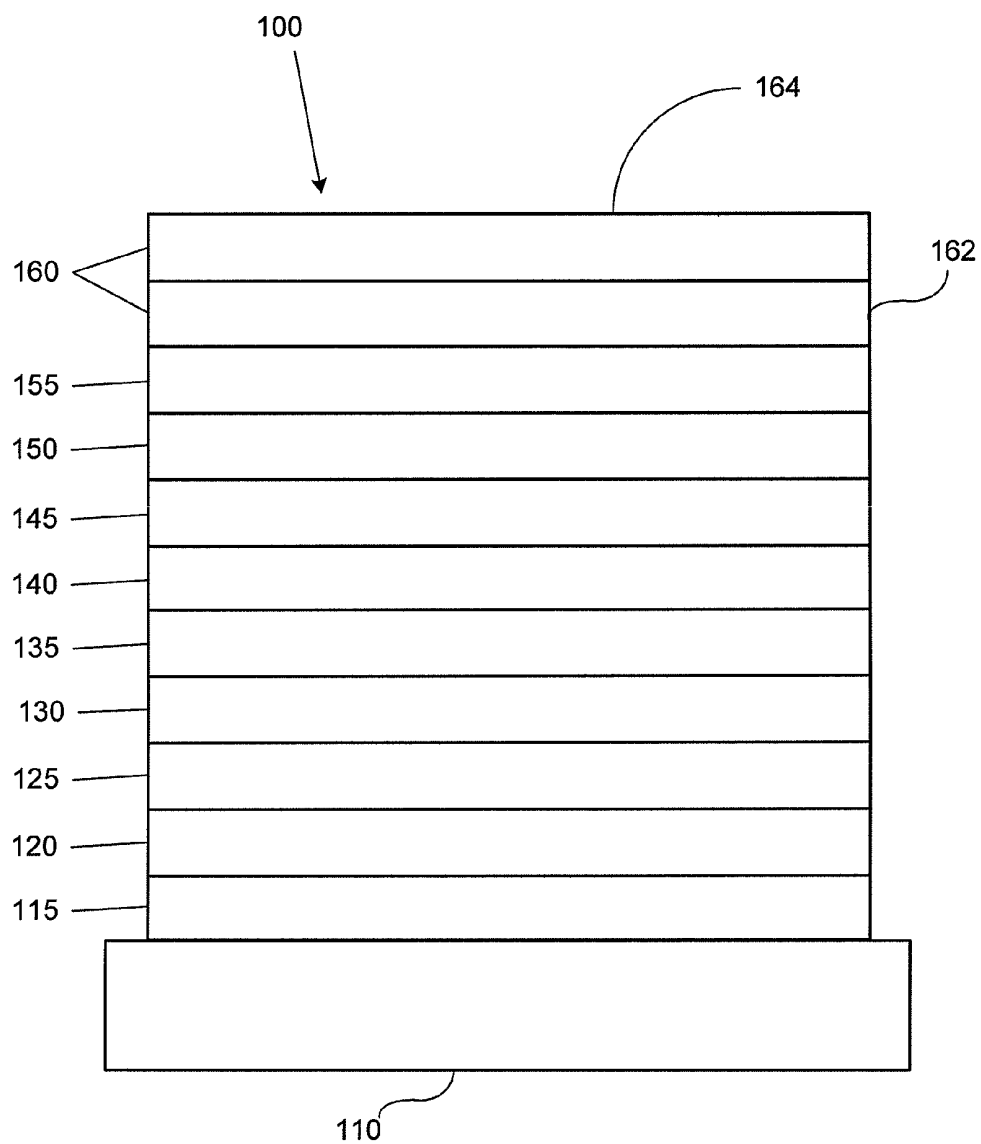


FIGURE 1

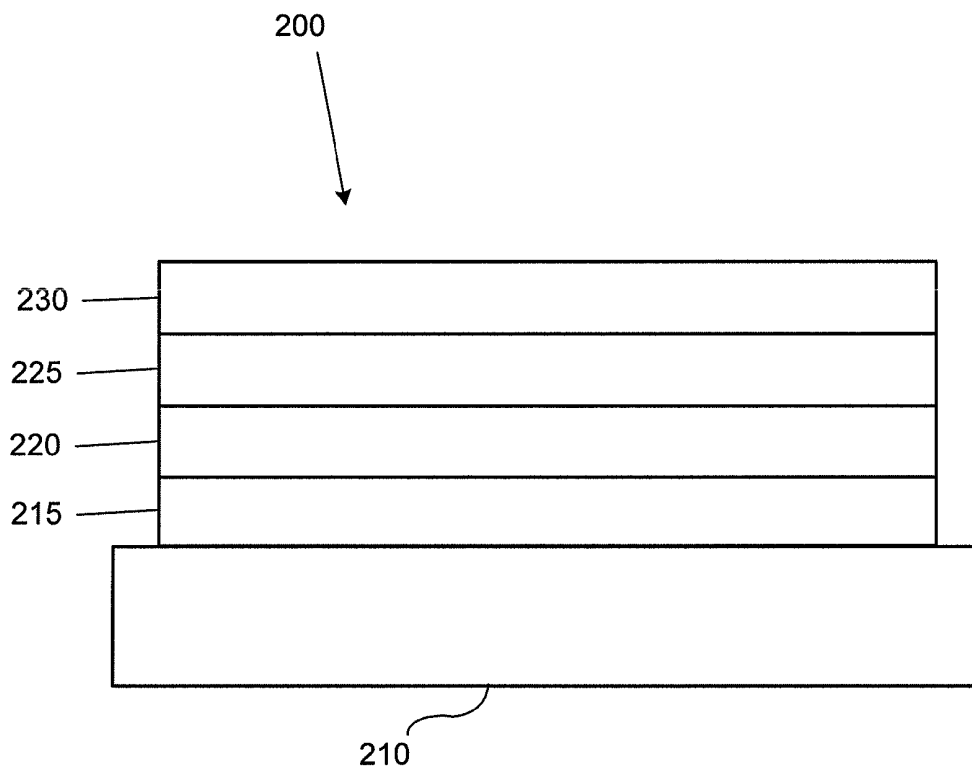


FIGURE 2

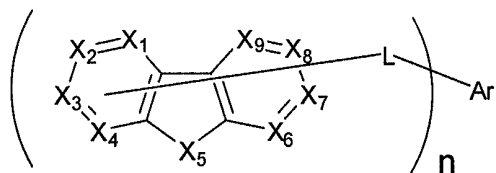


FIGURE 3

## ELECTRON TRANSPORTING COMPOUNDS

The claimed invention was made by, on behalf of, and/or in connection with one or more of the following parties to a joint university corporation research agreement: Regents of the University of Michigan, Princeton University, The University of Southern California, and the Universal Display Corporation. The agreement was in effect on and before the date the claimed invention was made, and the claimed invention was made as a result of activities undertaken within the scope of the agreement.

## FIELD OF THE INVENTION

The present invention relates to organic light emitting devices (OLEDs). More specifically, the present invention relates to phosphorescent materials comprising an azadibenzo moiety and a condensed aromatic moiety having at least three benzene rings. These materials may be used in OLEDs to provide devices having improved performance.

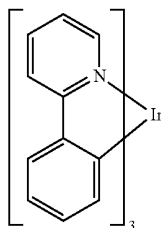
## BACKGROUND

Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer emits light may generally be readily tuned with appropriate dopants.

OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.

One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Color may be measured using CIE coordinates, which are well known to the art.

One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)<sub>3</sub>, which has the structure:



In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core moiety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule," and it is believed that all dendrimers currently used in the field of OLEDs are small molecules.

As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

As used herein, "solution processible" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level of the same material. A "higher" HOMO or LUMO energy level appears closer to the top of such a diagram than a "lower" HOMO or LUMO energy level.

As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a "higher" work function is more negative. On a conventional energy level diagram, with the vacuum level at the top, a "higher" work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

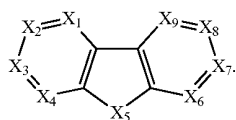
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More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

## SUMMARY OF THE INVENTION

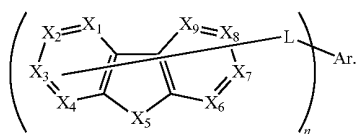
Compounds comprising an aza-dibenzo moiety and a condensed aromatic moiety having at least three benzene rings are provided. The compounds have the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$ .

Ar contains a condensed aromatic ring having at least three benzene rings and the condensed aromatic ring has a triplet energy lower than 440 nm. Ar is optionally further substituted. L is a single bond or a bivalent linking group. n is at least 1. i is an indexing variable that identifies n structures for  $\text{L}_i$  and  $\text{D}_i$  that may be the same or different for different values of i. Each  $\text{L}_i$  is independently a single bond or a bivalent linking group. Each  $\text{D}_i$  independently has the structure:



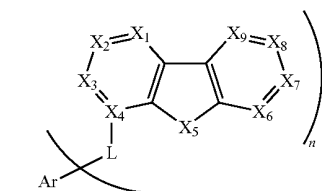
$\text{X}_5$  is O, S or Se. Each of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is independently selected from C(R) or N. At least one of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is N. Each R is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl. R is optionally bound to L.

In one aspect, the compound has the formula:

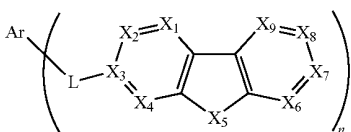


Formula I

In another aspect, the compound has a formula selected from the group consisting of:



Formula II

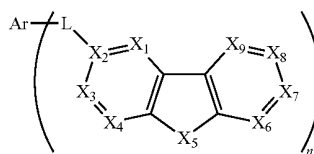


Formula III

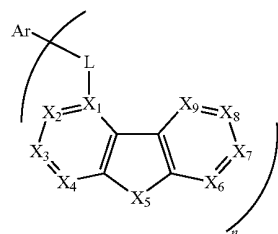
4

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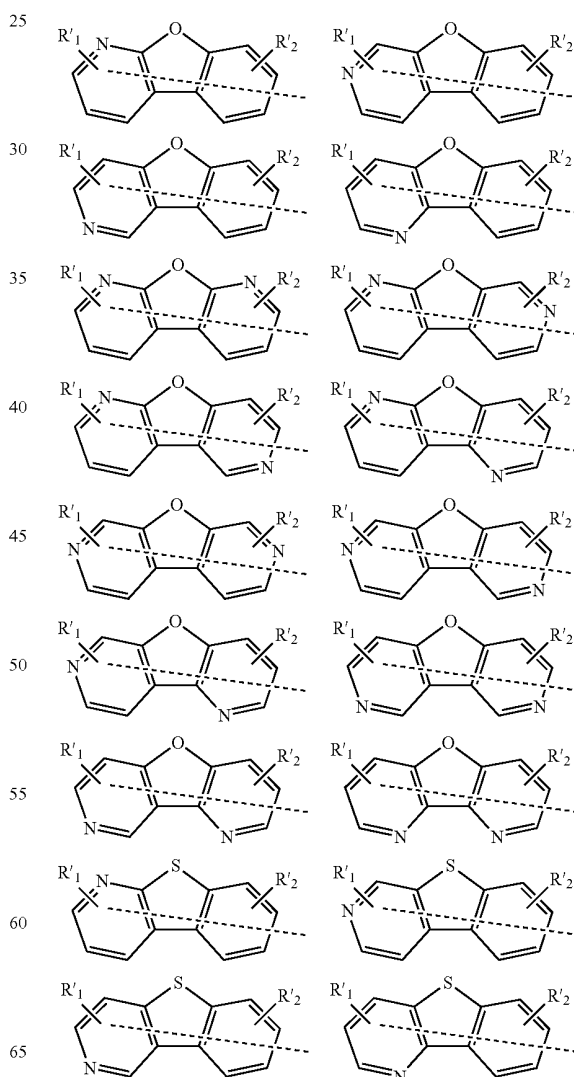
Formula IV



Formula V



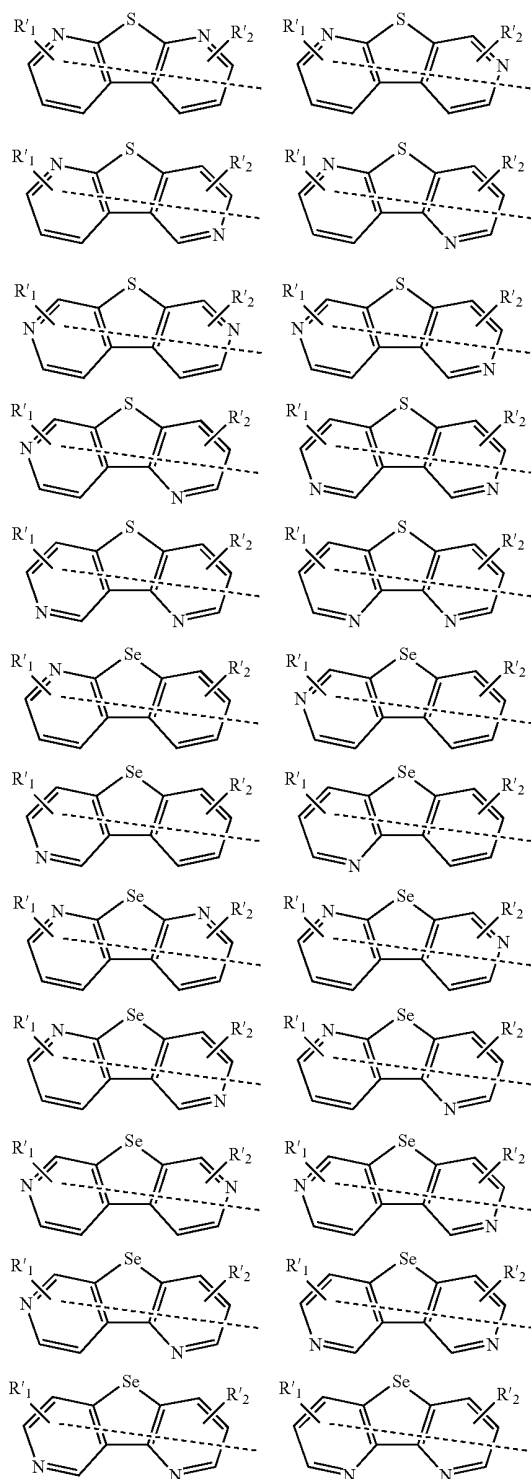
In one aspect, each  $\text{D}_i$  is independently selected from the group consisting of:





5

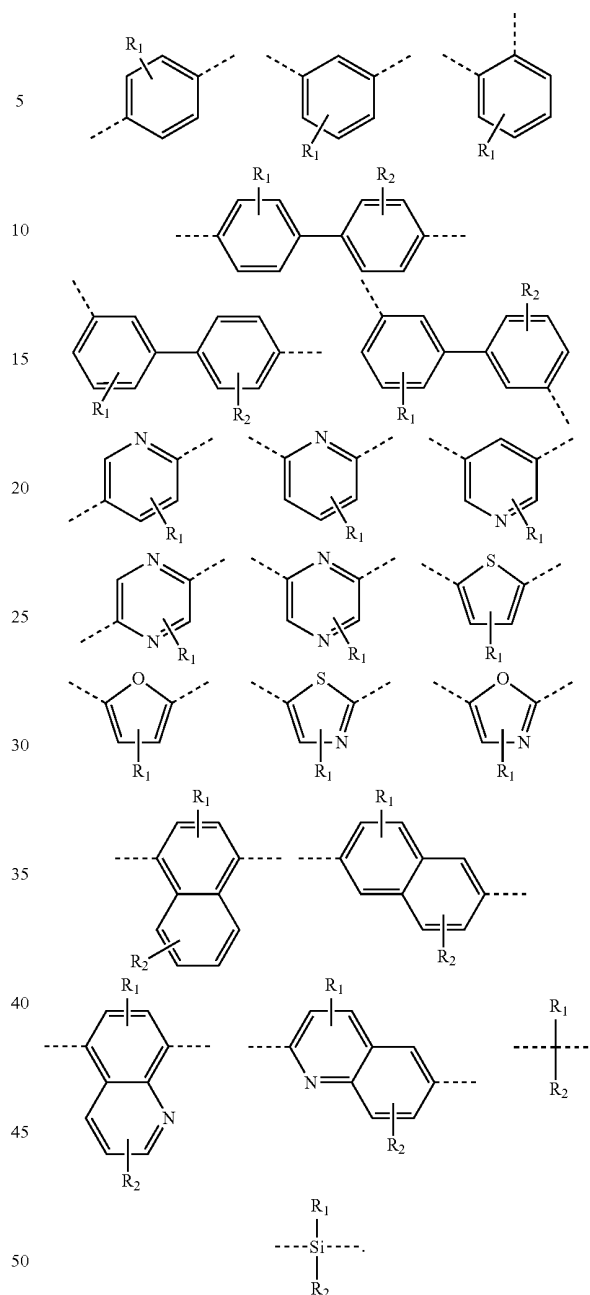
-continued



$R'_1$  and  $R'_2$  may represent mono, di, tri, or tetra substitutions.  $R'_1$  and  $R'_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect, L is a single bond. In another aspect, each  $L_i$  is independently selected from the group consisting of:

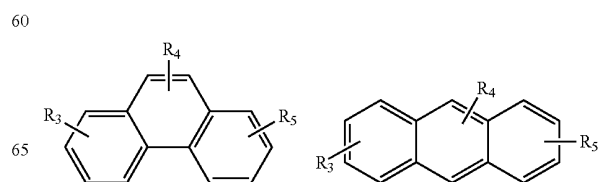
6



$R_1$  and  $R_2$  may represent mono, di, tri, or tetra substitutions.

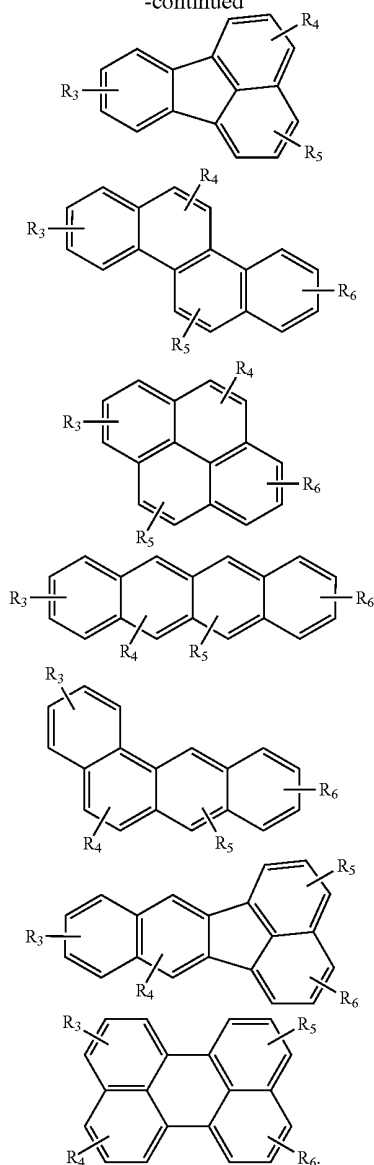
$R_1$  and  $R_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect, Ar is selected from the group consisting of:



7

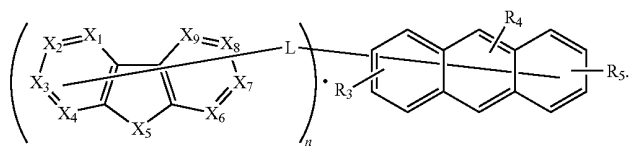
-continued



R<sub>3</sub>, R<sub>4</sub>, R<sub>5</sub> and R<sub>6</sub> may represent mono, di, tri, or tetra substitutions. R<sub>3</sub>, R<sub>4</sub>, R<sub>5</sub> and R<sub>6</sub> are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect, n is 1. In another aspect, n is greater than 1 and each D<sub>i</sub> has the same structure. In yet another aspect, n is greater than 1 and at least two D<sub>i</sub> have different structures. In a further aspect, n is 2.

Preferably, the compound has the formula:

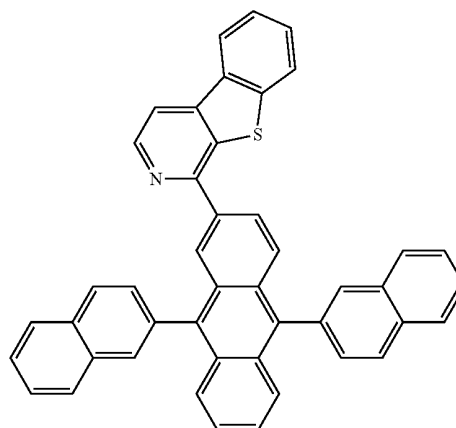


8

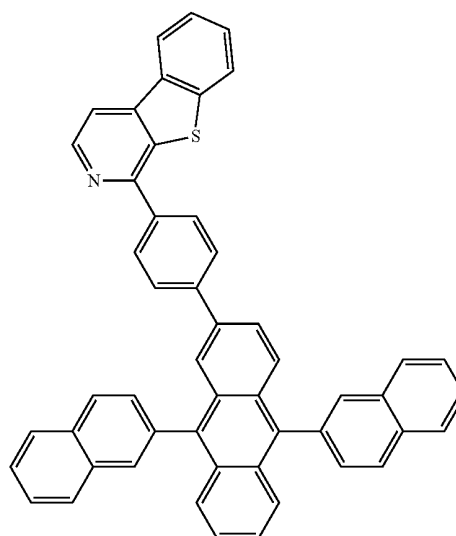
R<sub>3</sub>, R<sub>4</sub>, and R<sub>5</sub> may represent mono, di, tri, or tetra substitutions. R<sub>3</sub>, R<sub>4</sub>, and R<sub>5</sub> are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

Specific, non-limiting examples of the compounds comprising an aza-dibenzo moiety and an aromatic moiety having extended conjugation are provided. In one aspect, the compound is selected from the group consisting of:

Compound 1



Compound 2



Formula VI

9

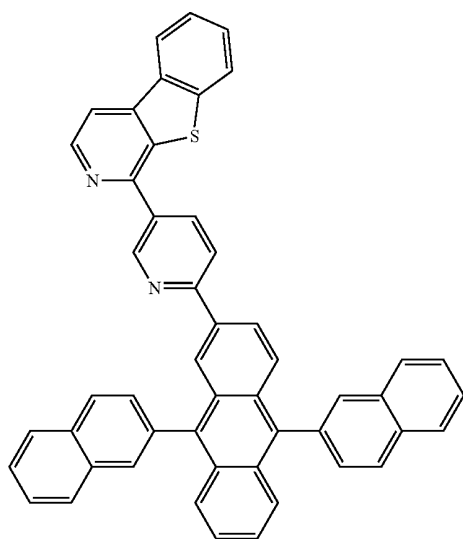
-continued

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Compound 5

Compound 3 5

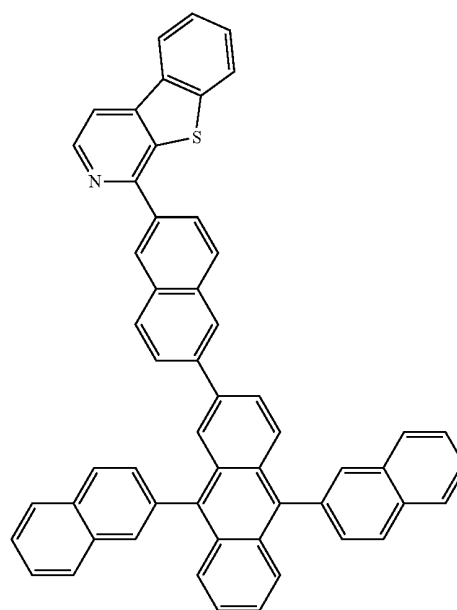


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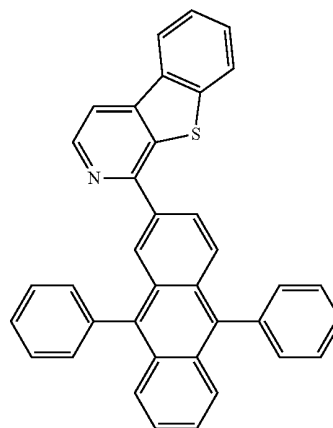
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Compound 6

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Compound 4



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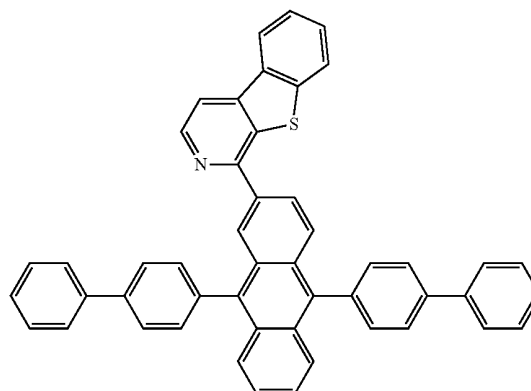
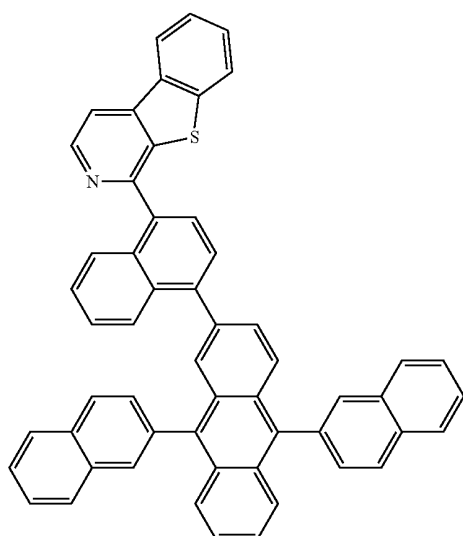
50

Compound 7

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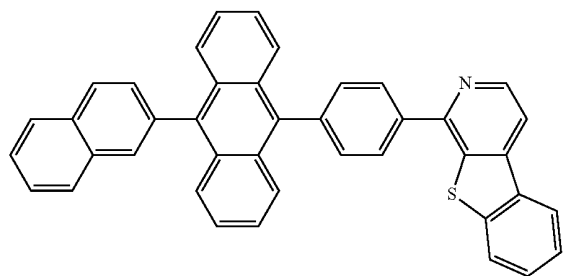
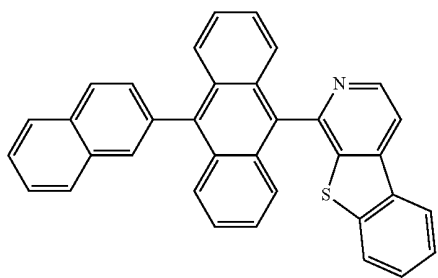
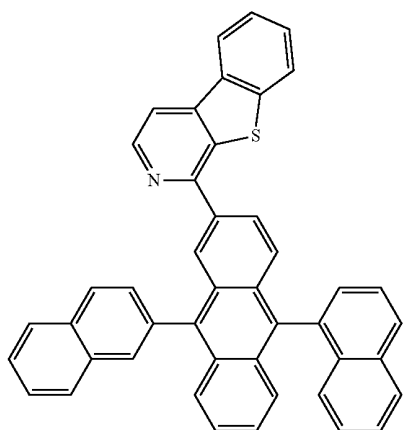
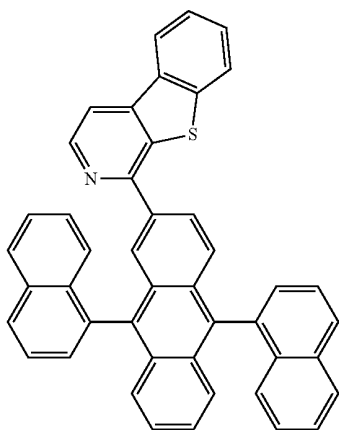
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11

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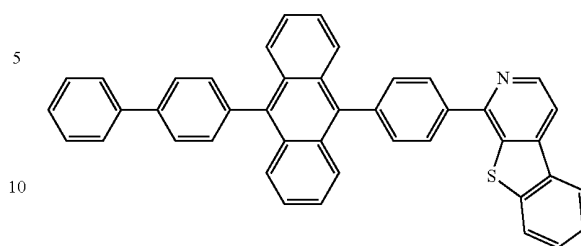


12

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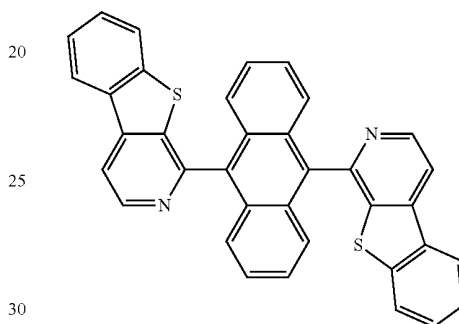
Compound 8

Compound 12



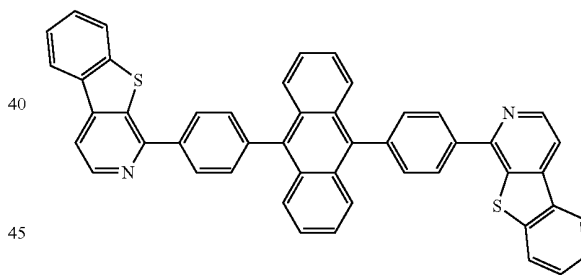
Compound 9

Compound 13



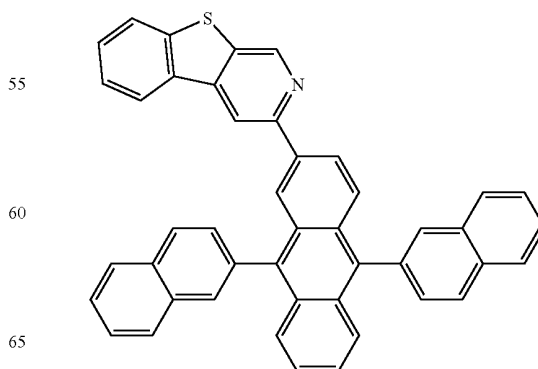
Compound 10

Compound 14



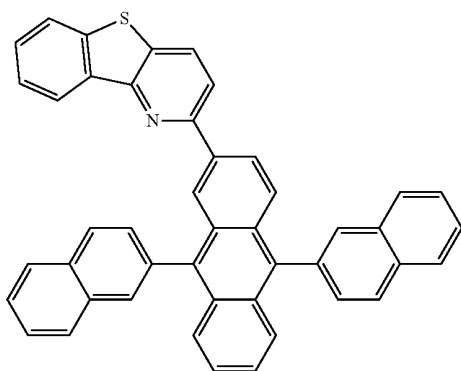
Compound 11

Compound 15



**13**

-continued



Compound 16

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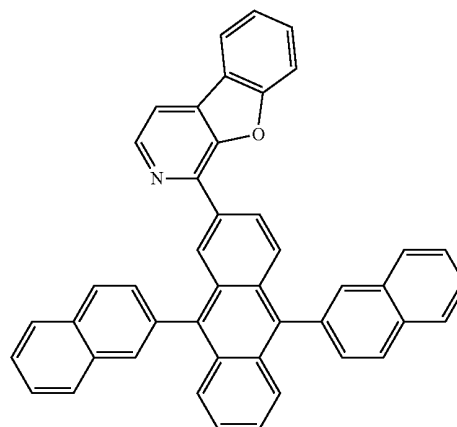
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**14**

-continued



Compound 19

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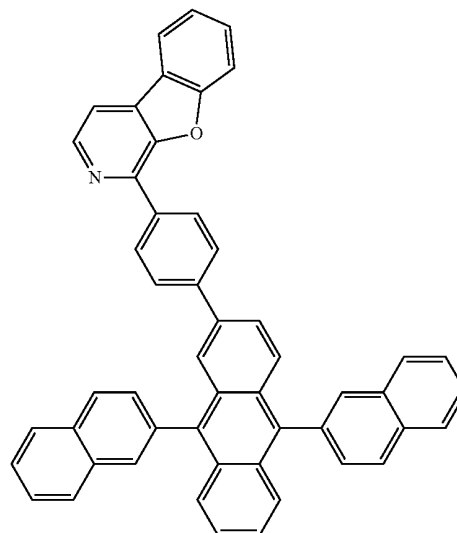
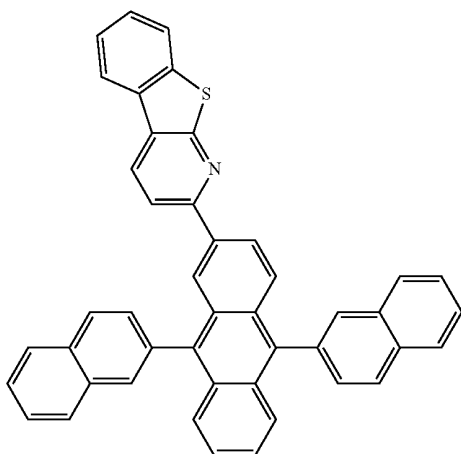
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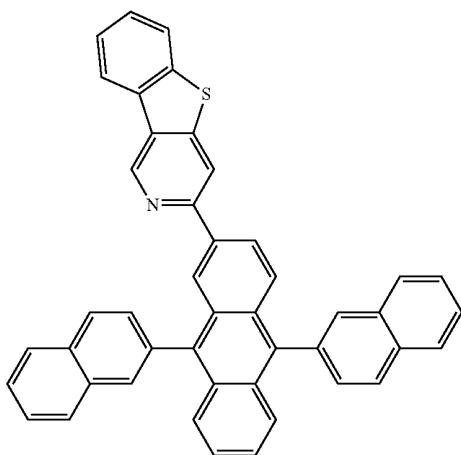
45

Compound 17



Compound 20

Compound 18

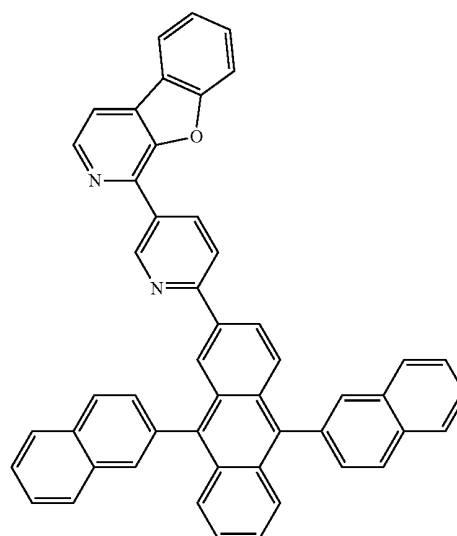


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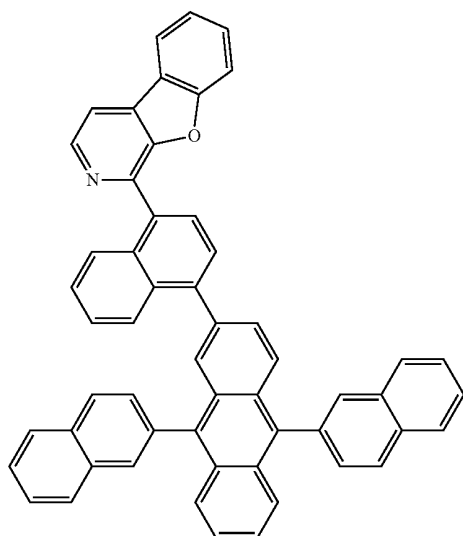
65



Compound 21

**15**

-continued



Compound 22

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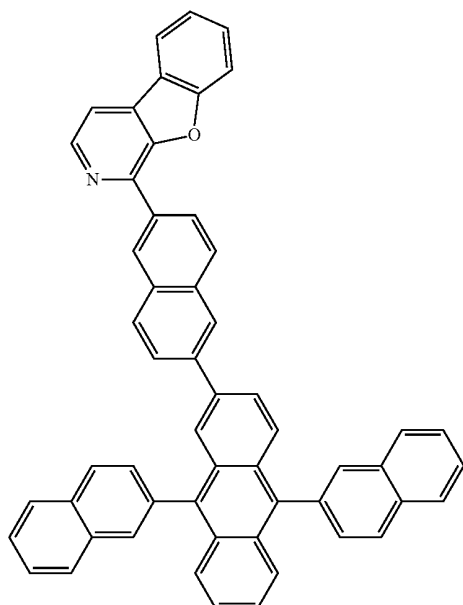
20

Compound 23

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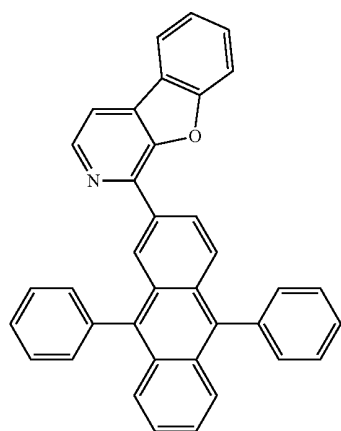
35



Compound 24

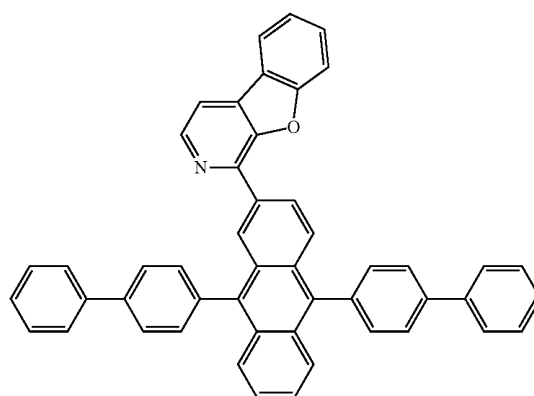
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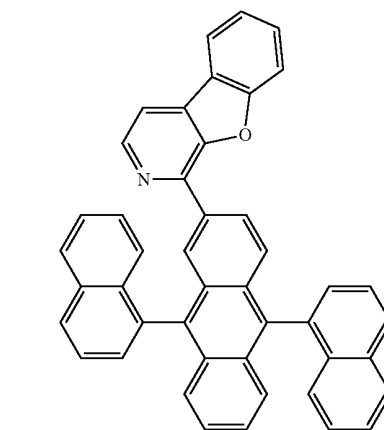
**16**

-continued

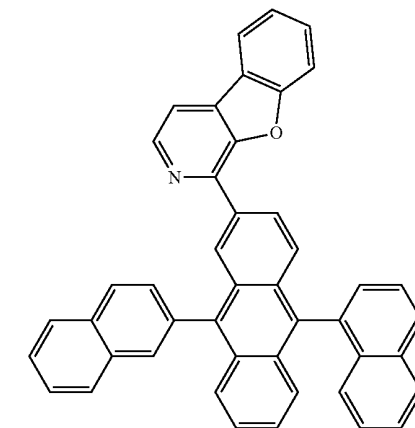


Compound 25

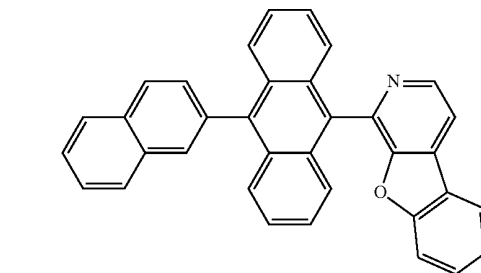
Compound 26



Compound 27



Compound 28

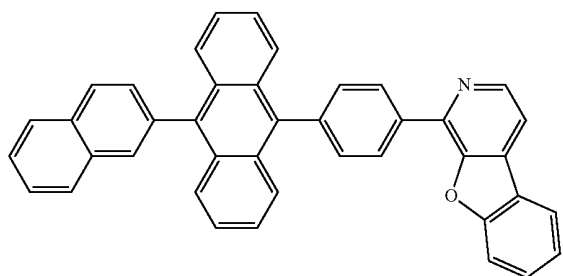


65

**17**

-continued

Compound 29



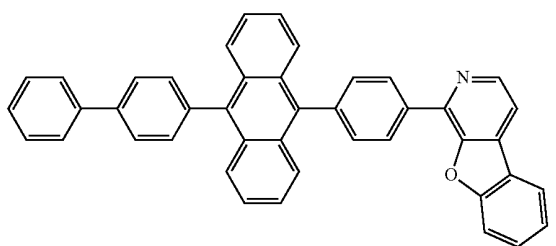
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Compound 30

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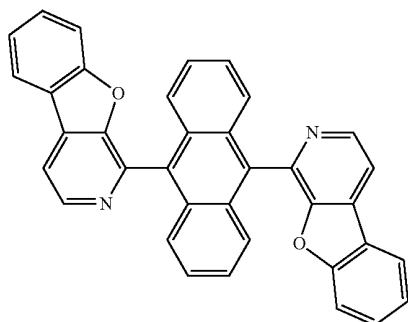


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Compound 31

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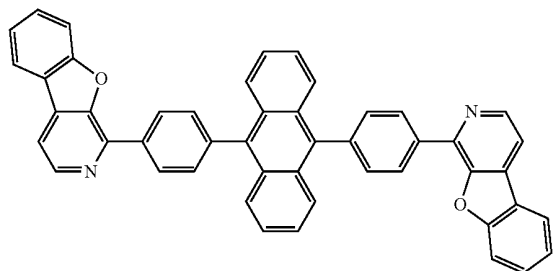


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Compound 32

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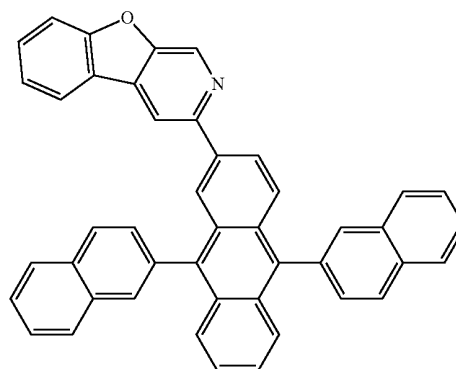
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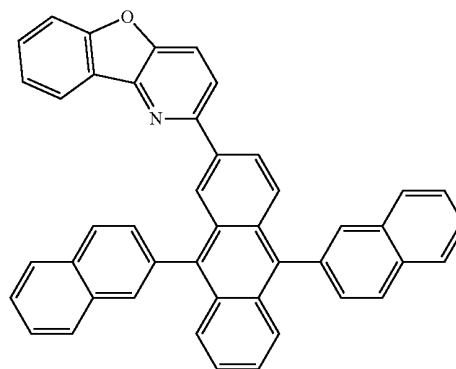
**18**

-continued

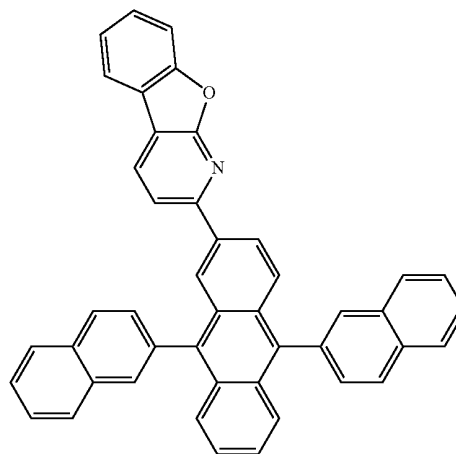
Compound 33



Compound 34

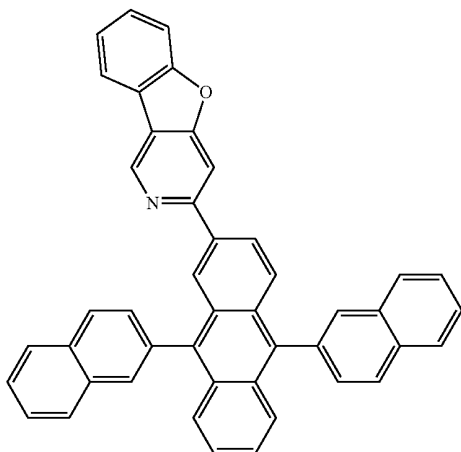


Compound 35



**19**  
-continued

Compound 36



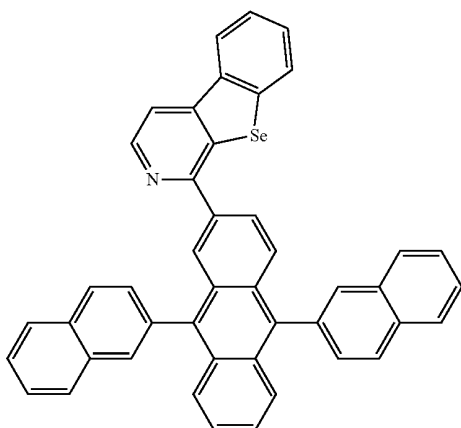
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Compound 37

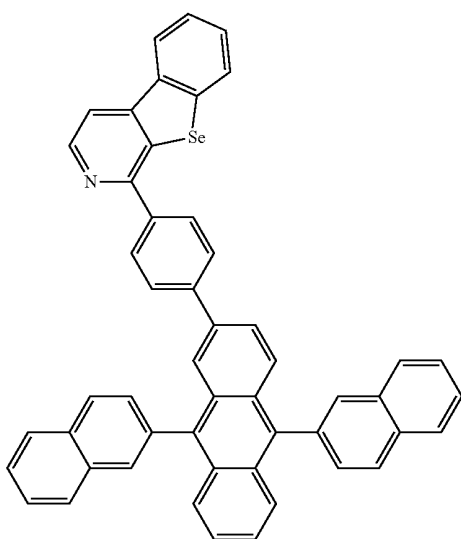


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Compound 38



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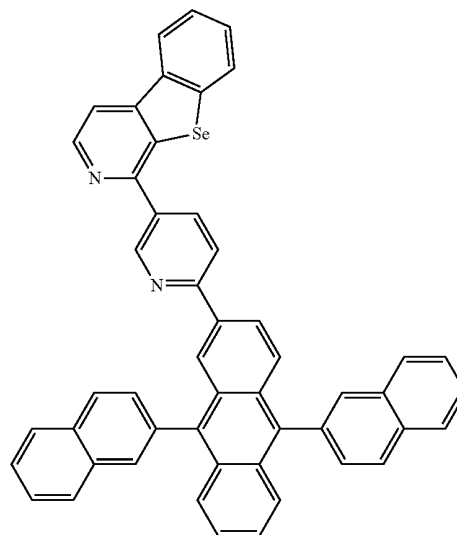
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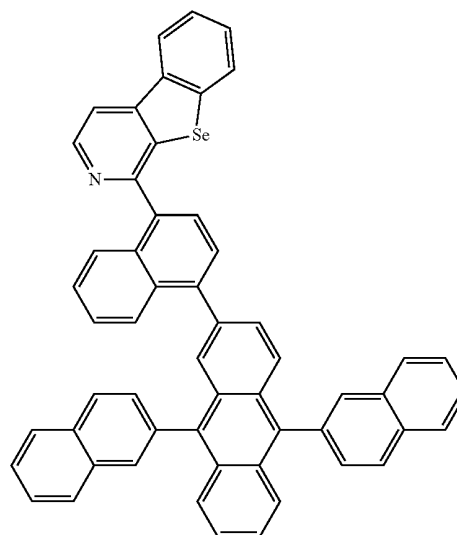
65

**20**  
-continued

Compound 39



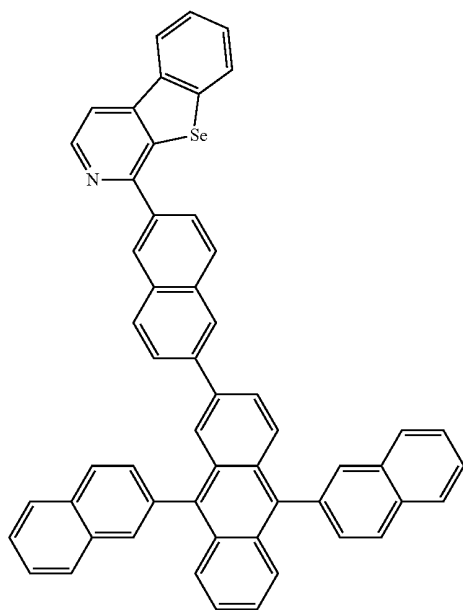
Compound 40





**21**

-continued



Compound 41

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Compound 42

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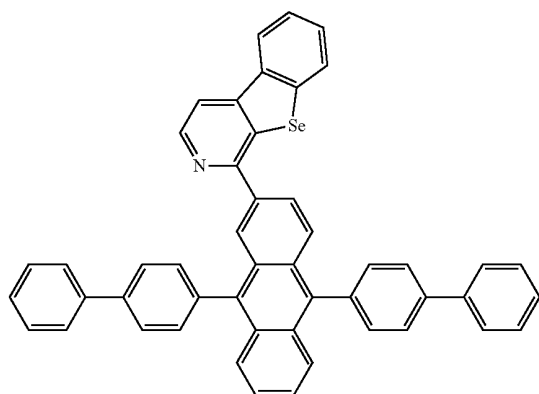
Compound 43

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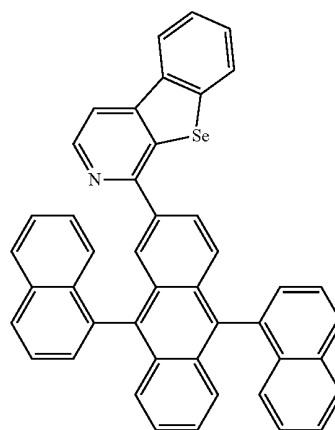
60

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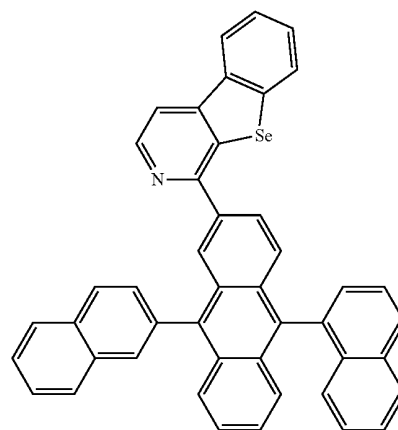
**22**

-continued

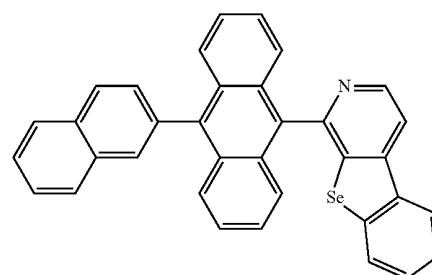


Compound 44

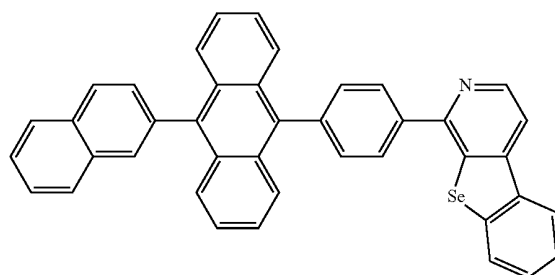
Compound 45



Compound 46



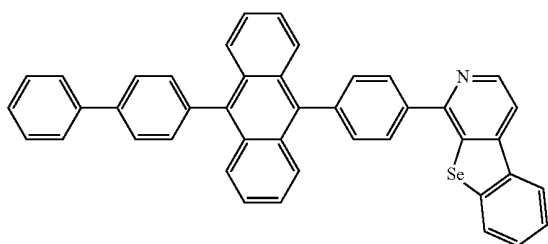
Compound 47



**23**

-continued

Compound 48

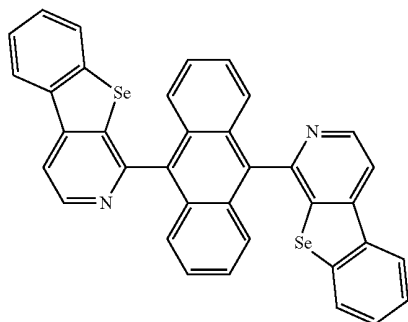


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Compound 49

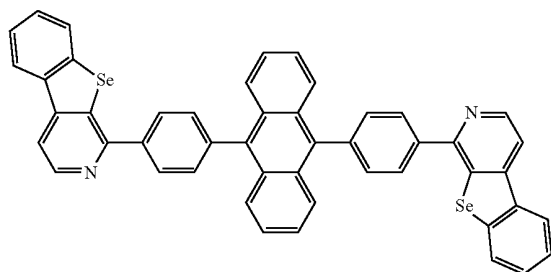


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Compound 50

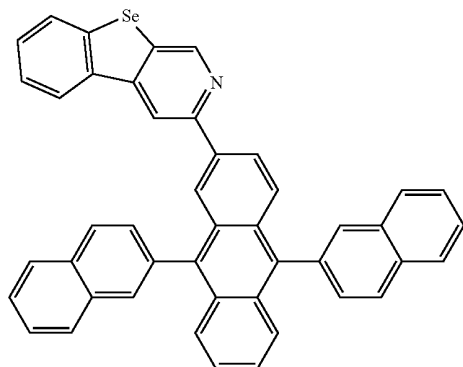


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Compound 51



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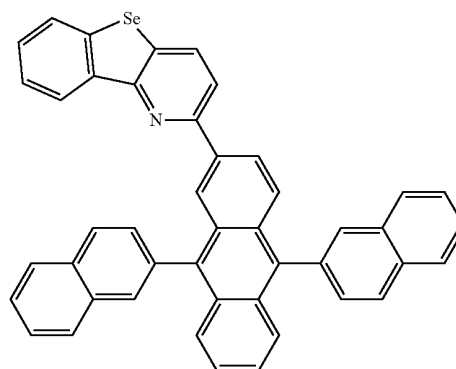
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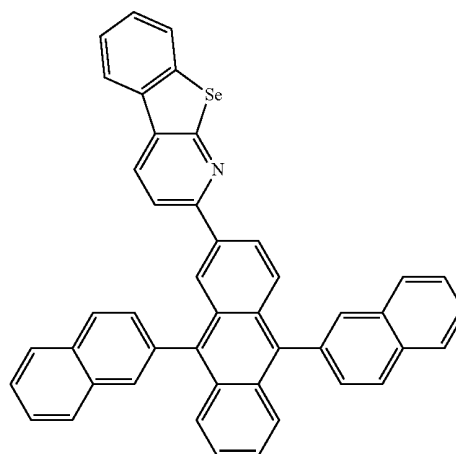
**24**

-continued

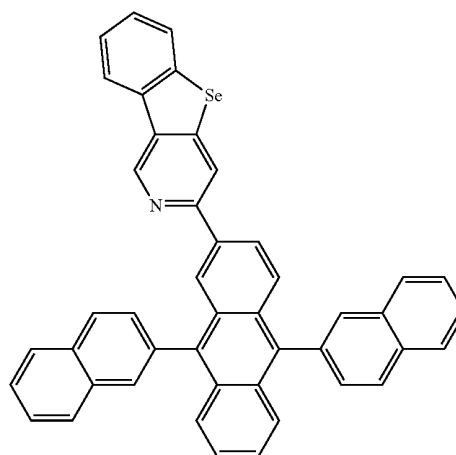
Compound 52



Compound 53



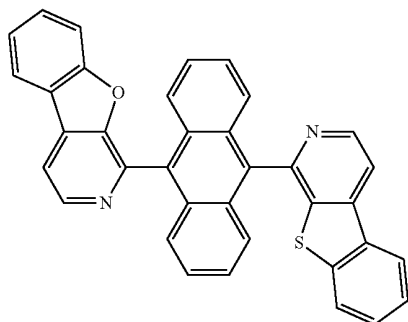
Compound 54



**25**

-continued

Compound 55

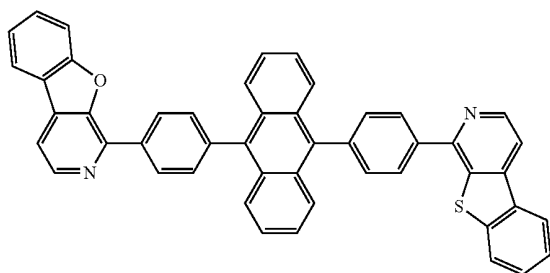


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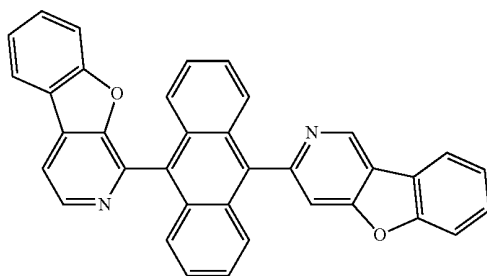
Compound 56



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Compound 57

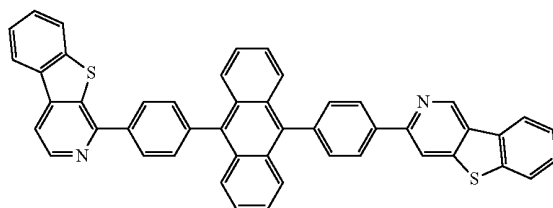


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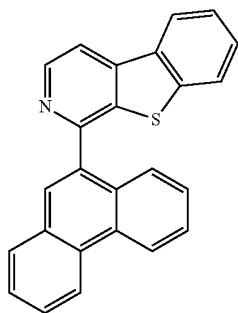
Compound 58



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Compound 59



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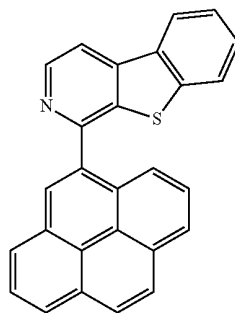
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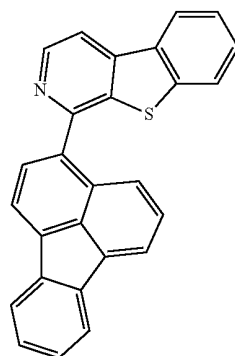
**26**

-continued

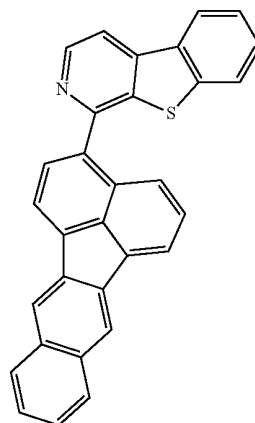
Compound 60



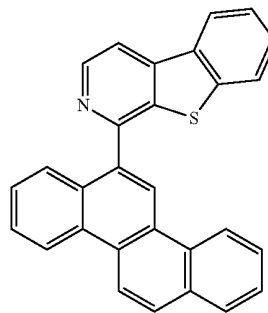
Compound 61



Compound 62

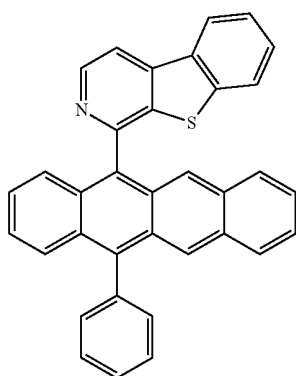


Compound 63

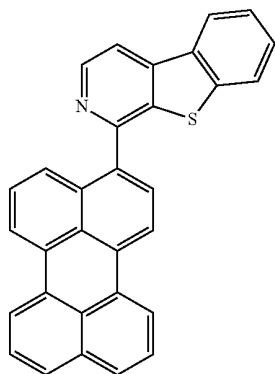


27

-continued



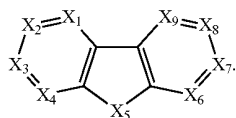
Compound 64



Compound 65

A first device comprising an organic light emitting device is also provided. The organic light emitting device comprises an anode, a cathode, and an organic layer that is disposed between the anode and the cathode. The organic layer comprises a compound having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$ .

Ar contains a condensed aromatic ring having at least three benzene rings and the condensed aromatic ring has a triplet energy lower than 440 nm. Ar is optionally further substituted. L is a single bond or a bivalent linking group. n is at least 1. i is an indexing variable that identifies n structures for  $\text{L}_i$  and  $\text{D}_i$  that may be the same or different for different values of i. Each  $\text{L}_i$  is independently a single bond or a bivalent linking group. Each  $\text{D}_i$  independently has the structure:



$\text{X}_5$  is O, S or Se. Each of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is independently selected from C(R) or N. At least one of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is N. Each R is independently

28

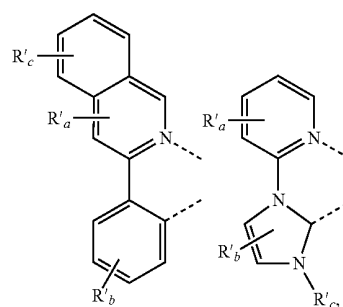
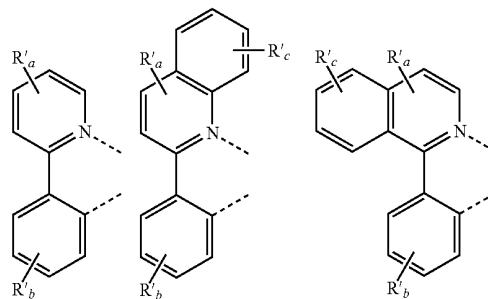
selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl. R is optionally bound to L.

The various specific aspects discussed above for compounds having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$  are also applicable to the compounds having formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$  when used in a first device. In particular, specific aspects of Ar, L, n,  $\text{D}_i$ ,  $\text{X}_1$ - $\text{X}_9$ , R,  $\text{R}'_1$ ,  $\text{R}'_2$ ,  $\text{R}_1$ - $\text{R}_6$ , Formula I, Formula II, Formula III, Formula IV, Formula V and Formula VI of the compounds having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$ , as discussed above, are also applicable to a compound having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$  that is used in the first device.

Specific, non-limiting examples of devices comprising the compounds disclosed herein are provided. In one aspect, the compound used in the first device is selected from the group consisting of Compound 1-Compound 65.

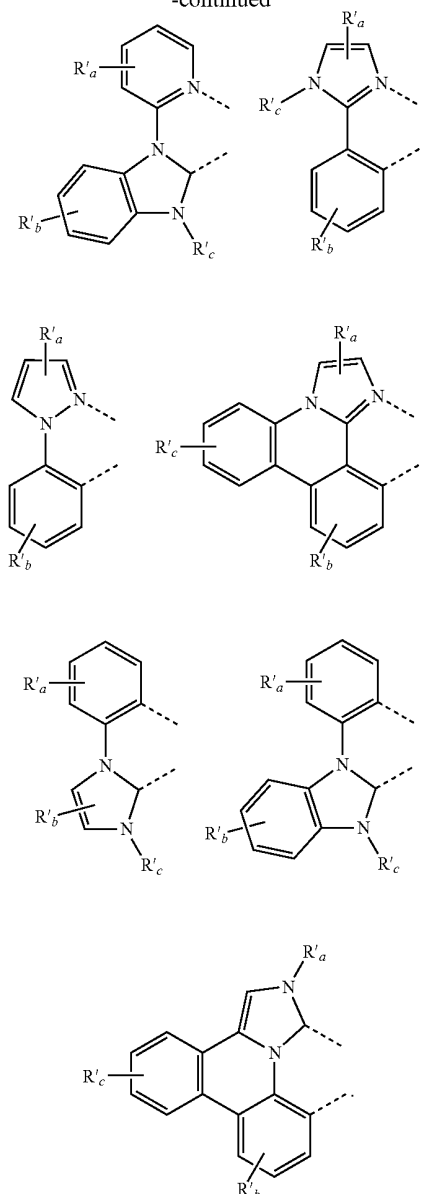
In one aspect, the organic layer is a non-emissive layer and the compound is a non-emissive compound. In another aspect, the organic layer is an electron transport layer and the compound is an electron transport material. In yet another aspect, the electron transport layer is doped with an n-type conductivity dopant. In one aspect, the n-type conductivity dopant is a compound containing Li, Na, K, Rb, or Cs. Preferably, the n-type conductivity dopant is selected from the group consisting of LiF, CsF, NaCl, KBr, and LiQ.

In another aspect, the organic layer further comprises an emissive compound that is a transition metal complex having at least one ligand selected from the group consisting of:



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-continued



Each of R'<sub>a</sub>, R'<sub>b</sub> and R'<sub>c</sub> may represent mono, di, tri, or tetra substituents. Each of R'<sub>a</sub>, R'<sub>b</sub> and R'<sub>c</sub> are independently selected from a group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, or heteroaryl. Two adjacent substituents may form into a ring.

In one aspect, the first device is a consumer product. In another aspect, the first device is an organic light emitting device.

#### BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 shows an organic light emitting device.

FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

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FIG. 3 shows an exemplary compound comprising an azabenzido moiety and an aromatic moiety having extended conjugation.

#### DETAILED DESCRIPTION

Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, an "exciton," which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

The initial OLEDs used emissive molecules that emitted light from their singlet states ("fluorescence") as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," *Nature*, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," *Appl. Phys. Lett.*, vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

FIG. 1 shows an organic light emitting device 100. The figures are not necessarily drawn to scale. Device 100 may include a substrate 110, an anode 115, a hole injection layer 120, a hole transport layer 125, an electron blocking layer 130, an emissive layer 135, a hole blocking layer 140, an electron transport layer 145, an electron injection layer 150, a protective layer 155, and a cathode 160. Cathode 160 is a compound cathode having a first conductive layer 162 and a second conductive layer 164. Device 100 may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F.sub.4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use

of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

FIG. 2 shows an inverted OLED 200. The device includes a substrate 210, a cathode 215, an emissive layer 220, a hole transport layer 225, and an anode 230. Device 200 may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device 200 has cathode 215 disposed under anode 230, device 200 may be referred to as an "inverted" OLED. Materials similar to those described with respect to device 100 may be used in the corresponding layers of device 200. FIG. 2 provides one example of how some layers may be omitted from the structure of device 100.

The simple layered structure illustrated in FIGS. 1 and 2 is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device 200, hole transport layer 225 transports holes and injects holes into emissive layer 220, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.

Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. patent application Ser. No. 10/233,470, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processibility than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.).

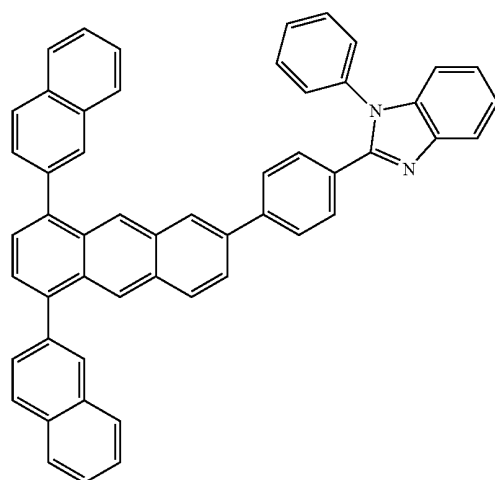
The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, arylkyl, heterocyclic group, aryl, aromatic group, and heteroaryl are known to the art, and are defined in U.S. Pat. No. 7,279,704 at cols. 31-32, which are incorporated herein by reference.

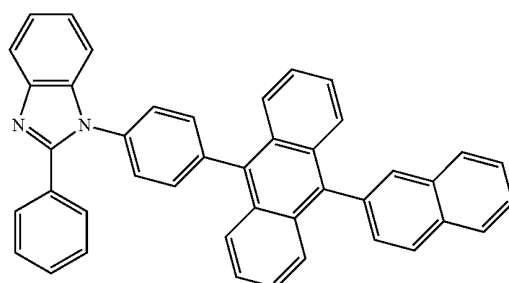
Various materials have been reported for use in the electron transport layer (ETL) of OLEDs. For example, anthracene-benzimidazole compounds, azatriphenylene derivatives, anthracene-benzothiazole compounds, and metal 8-hydroxyquinolates are all commonly used electron transporting materials. Table 1 summarizes several commonly used electron transporting materials.

TABLE 1

Anthracene-  
benzimidazole  
compounds

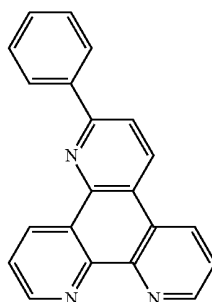


WO2003060956



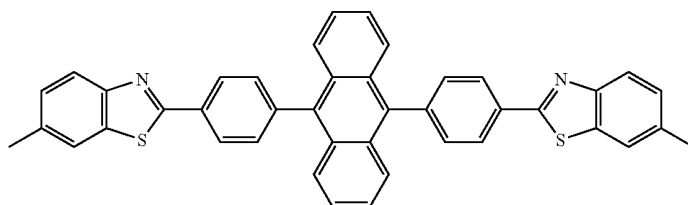
U.S. Pat. No.  
20090179554

Aza triphenylene  
derivatives



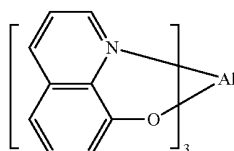
U.S. Pat. No.  
20090115316

Anthracene-  
benzothiazole  
compounds



Appl. Phys. Lett. 89,  
063504 (2006)

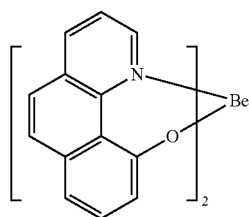
Metal 8-hydroxy-  
quinolates  
(e.g., Alq<sub>3</sub>, Zr<sub>q</sub><sub>4</sub>)



Appl. Phys. Lett. 51,  
913 (1987)  
U.S. Pat. No.  
7230107

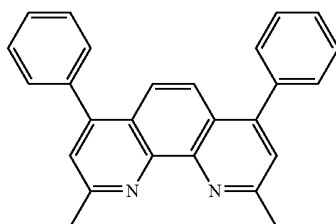
TABLE 1-continued

Metal  
hydroxy-  
benoquinolates

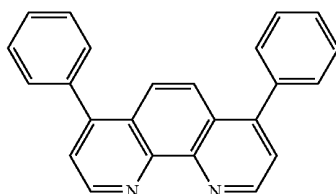


Chem. Lett. 5, 905  
(1993)

Bathocuprine  
compounds  
such as BCP,  
BPhen, etc

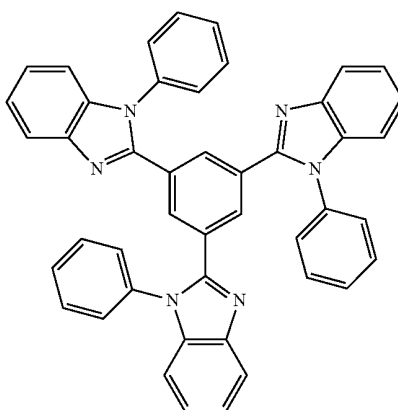


Appl. Phys. Lett. 91,  
263503 (2007)

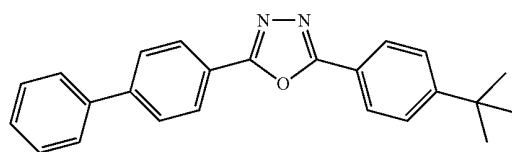


Appl. Phys. Lett. 79,  
449 (2001)

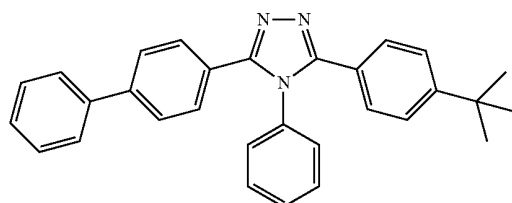
5-member ring  
electron deficient  
heterocycles  
(e.g., triazole,  
oxadiazole,  
imidazole,  
benzimidazole)



Appl. Phys. Lett. 74,  
865 (1999)



Appl. Phys. Lett. 55,  
1489 (1989)



Jpn. J. Apply. Phys.  
32, L917 (1993)



TABLE 1-continued

Silole compounds

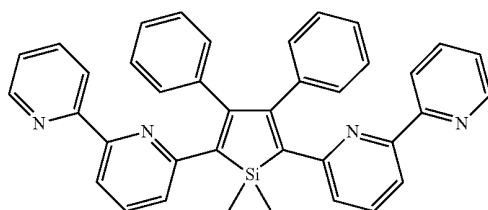
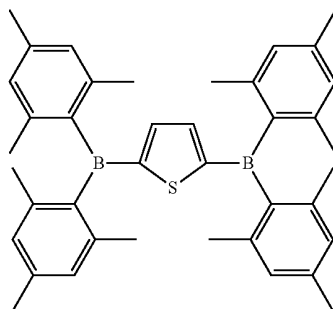
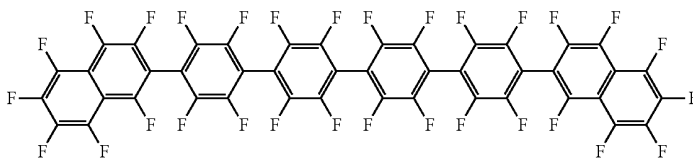
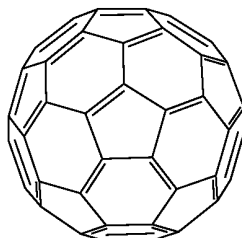
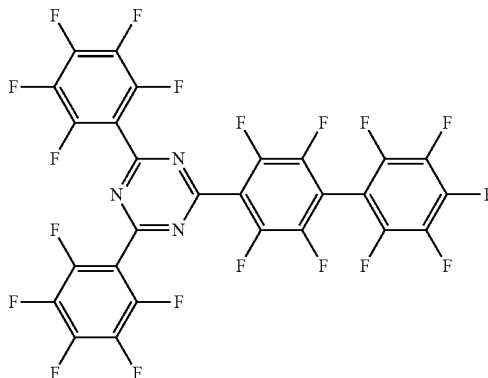
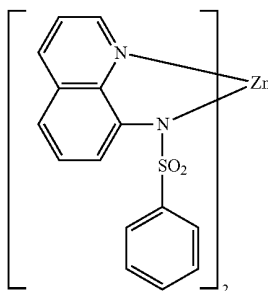
Org. Electron. 4, 13  
(2003)Arylborane  
compoundsJ. Am. Chem. Soc.  
120, 9714 (1998)Fluorinated  
aromatic  
compoundsJ. Am. Chem. Soc.  
122, 1832 (2000)Fullerene  
(e.g., C60)U.S. Pat. No.  
20090101870Triazine  
complexesU.S. Pat. No.  
20040036077

TABLE 1-continued

Zn (N<sup>+</sup>N)  
complexesU.S. Pat. No.  
6528187

15

Even though many materials have been reported for use as an ETL material, the development a device with low operating voltage and good stability has remained problematic. Alq is a commonly used ETL material, but Alq has limitations for use in OLEDs. While Alq may have good stability, devices comprising Alq may have high operating voltage due to low electron mobility. Anthracene compounds with benzimidazole substituents have also been reported as ETL materials. See, e.g., U.S. Pat. No. 6,878,469 and US20090179554. However, these compounds may also have limitations when used as an ETL material in a device. Introducing electron deficient heterocycles, such as benzimidazole, oxadiazole, triazole, triazine, and pyridine, may increase electron affinity thereby resulting in good electron transporting properties and lowered device voltage, but often these compounds provide reduced device lifetime, too.

It is very difficult to predict whether the additional of electron deficient groups will result in improved device properties. For example, devices comprising an anthracene compound with a benzimidazole substituent may have reasonable device lifetime and operating voltage, as compared to devices using Alq as an ETL material; however, devices that use these electron deficient heterocyclic compounds in the ETL often have very short lifetimes. For example, devices using 1,3,5-tris(1-phenyl-1H-benzo[d]imidazol-2-yl)benzene (TPBi) as the ETL material have good efficiency, but very poor lifetime. Therefore, it is very difficult to predict which compounds may provide a low operating voltage and a long device lifetime.

Azadibenzofurans, azadibenzothiophenes, and azadibenzoselenophenes have been used as building blocks for host materials in phosphorescent OLEDs. See, JP2008074939. These materials have lower LUMOs, i.e., better electron affinity, than the corresponding dibenzofurans, dibenzothiophenes, and dibenzoselenophenes. It is believed that the electron affinity of these aza heterocyclic compounds may be advantageously used in ETL materials.

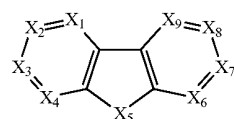
The compounds provided herein comprise an aromatic moiety with condensed aromatic rings with a low triplet energy and an aza-dibenzo moiety. By combining the aza-dibenzo moiety, e.g., azadibenzofuran, azadibenzothiophene, and azadibenzoselenophene, and the aromatic moiety, e.g., anthracene, in a compound, the result is ETL materials providing low voltage and good device stability. In particular, the compounds provided herein include anthracene compounds substituted with azadibenzofuran, azadibenzothiophene, or azadibenzoselenophene. These compounds may be used as

ETL materials in OLEDs to provide devices with lower operating voltage while maintaining good device stability. Without being bound by theory, it is believed that the aza-dibenzo moiety of the compound improves device voltage by reducing the LUMO and the aromatic moiety having a low triplet energy, i.e., higher conjugation, improves device stability by delocalizing and destabilizing the electron.

Additionally, the ETL materials provided herein can be doped with n-type conductivity dopants, e.g., LiF, CsF, NaCl, KBr, and LiQ.

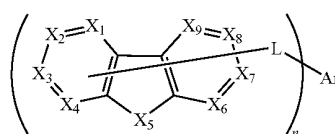
Compounds comprising an aza-dibenzo moiety and a condensed aromatic moiety having at least three benzene rings are provided. The compounds have the formula  $Ar(L_iD_i)_n$ .

Ar contains a condensed aromatic ring having at least three benzene rings and the condensed aromatic ring has a triplet energy lower than 440 nm. Ar is optionally further substituted. L is a single bond or a bivalent linking group. n is at least 1. i is an indexing variable that identifies n structures for  $L_i$  and  $D_i$  that may be the same or different for different values of i. Each  $L_i$  is independently a single bond or a bivalent linking group. Each  $D_i$  independently has the structure:



$X_5$  is O, S or Se. Each of  $X_1, X_2, X_3, X_4, X_6, X_7, X_8$ , and  $X_9$  is independently selected from C(R) or N. At least one of  $X_1, X_2, X_3, X_4, X_6, X_7, X_8$ , and  $X_9$  is N. Each R is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl. R is optionally bound to L.

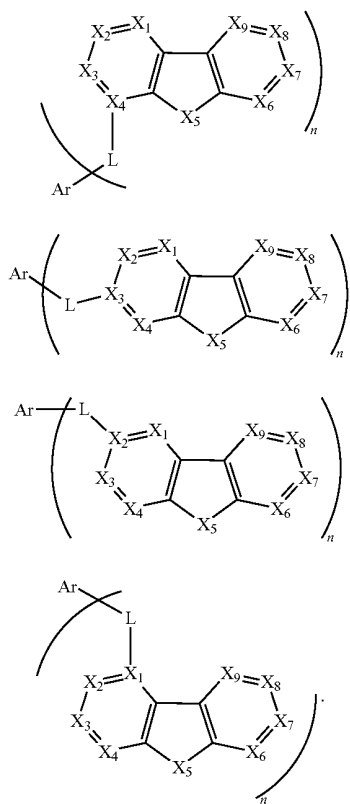
In one aspect, the compound has the formula:



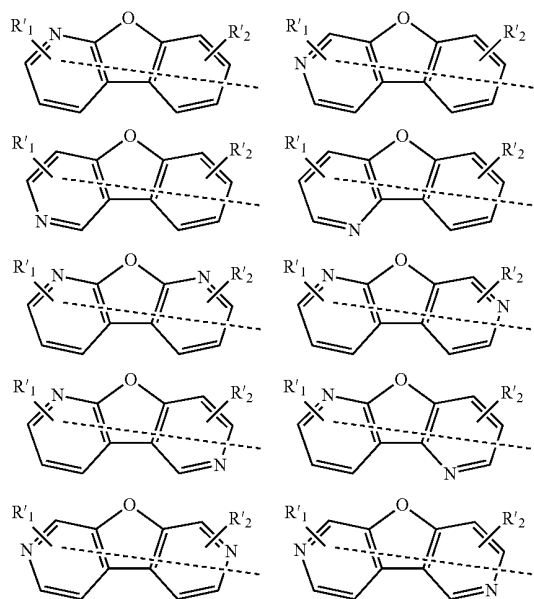
Formula I

41

In another aspect, the compound has a formula selected from the group consisting of:

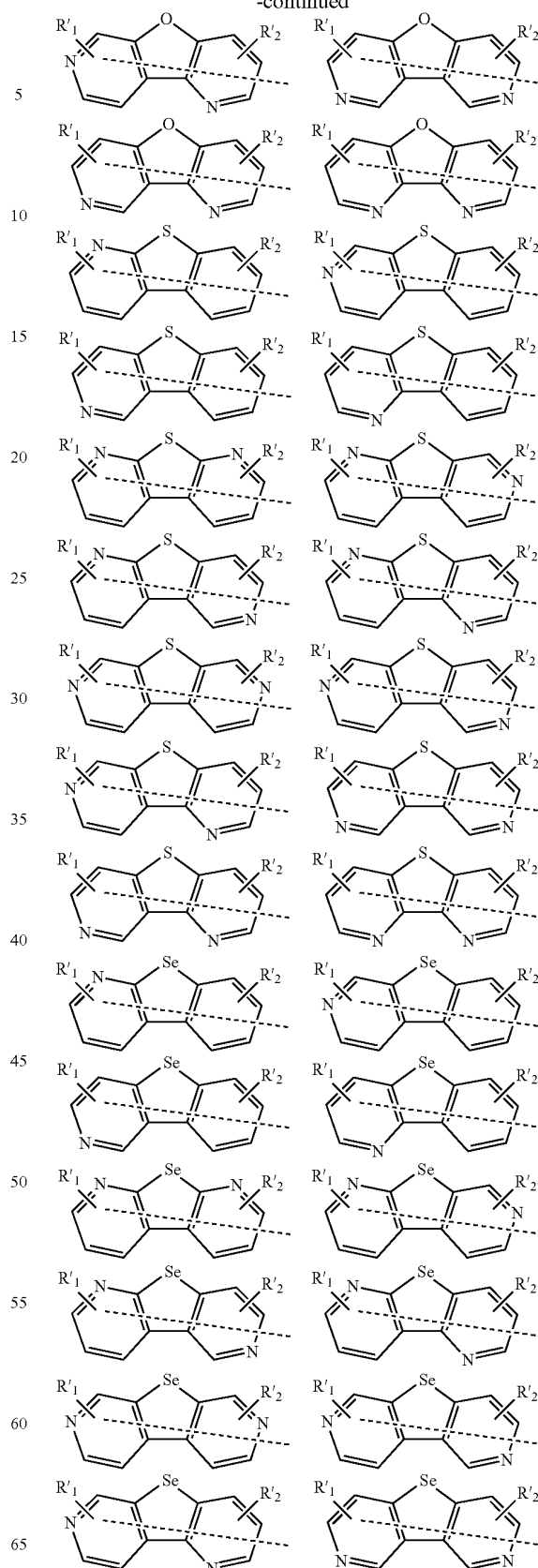


In one aspect, each  $D_i$  is independently selected from the group consisting of:

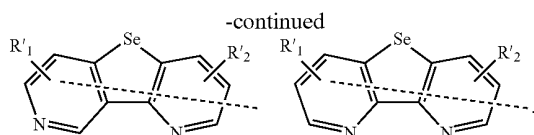


42

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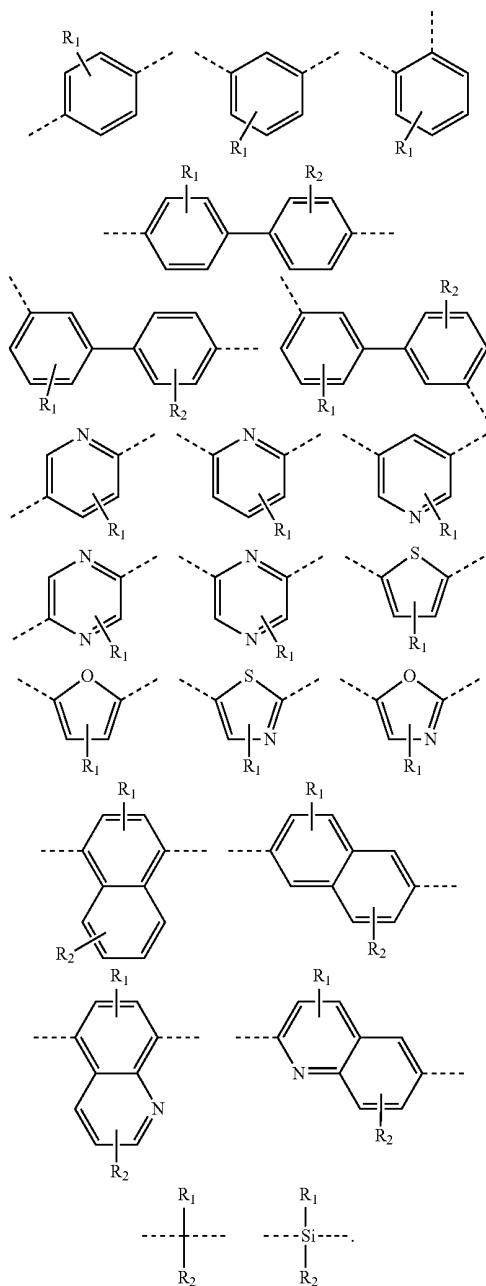


43



$R'_1$  and  $R'_2$  may represent mono, di, tri, or tetra substitutions.  $R'_1$  and  $R'_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

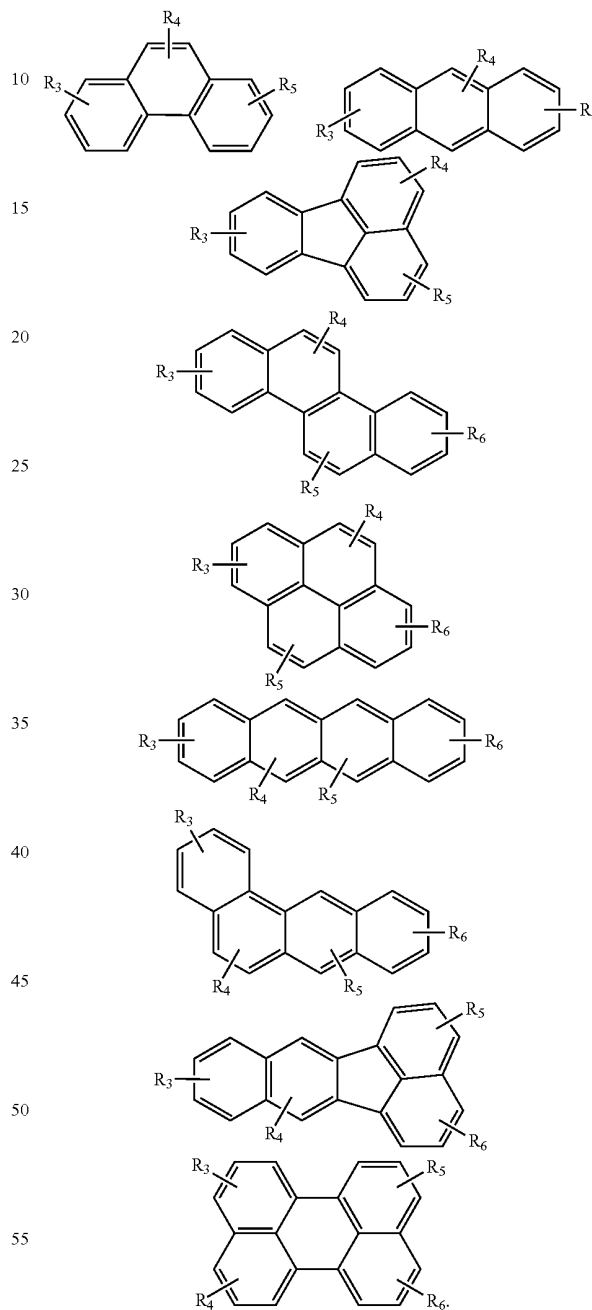
In one aspect,  $L$  is a single bond. In another aspect, each  $L_i$  is independently selected from the group consisting of:



44

$R_1$  and  $R_2$  may represent mono, di, tri, or tetra substitutions.  $R_1$  and  $R_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect,  $Ar$  is selected from the group consisting of:

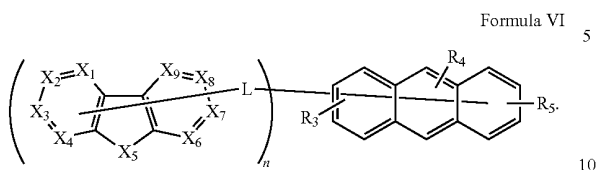


$R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  may represent mono, di, tri, or tetra substitutions.  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect,  $n$  is 1. In another aspect,  $n$  is greater than 1 and each  $D_i$  has the same structure. In yet another aspect,  $n$  is greater than 1 and at least two  $D_i$  have different structures. In a further aspect,  $n$  is 2.

**45**

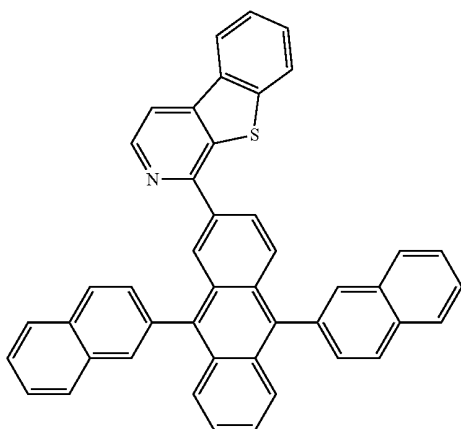
Preferably, the compound has the formula:



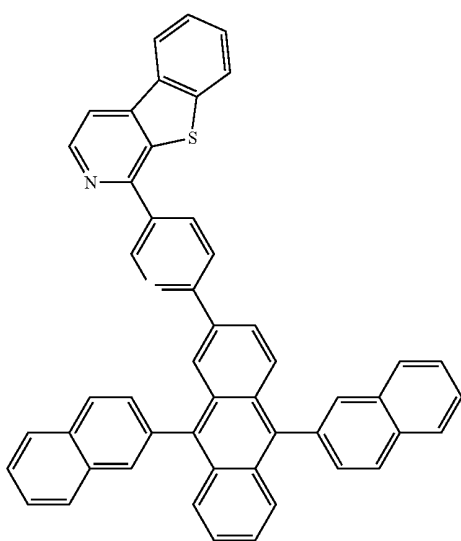
$R_3$ ,  $R_4$ , and  $R_5$  may represent mono, di, tri, or tetra substitu- 15  
 tions.  $R_3$ ,  $R_4$ , and  $R_5$  are independently selected from the  
 group consisting of hydrogen, deuterium, alkyl, alkoxy,  
 amino, silyl, cyano, halogen, aryl, and heteroaryl.

Specific, non-limiting examples of the compounds comprising an aza-dibenzo moiety and an aromatic moiety having 20  
 extended conjugation are provided. In one aspect, the compound is selected from the group consisting of:

Compound 1

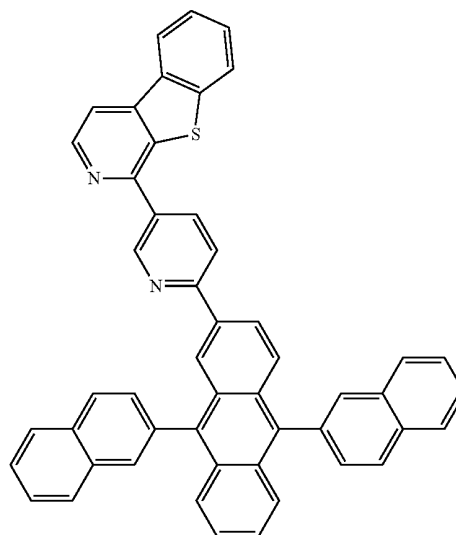


Compound 2

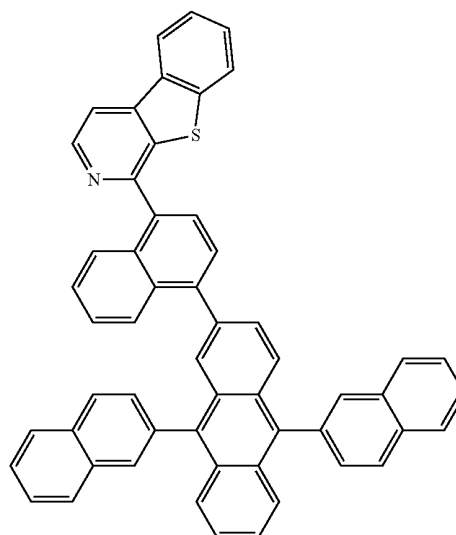
**46**

-continued

Compound 3

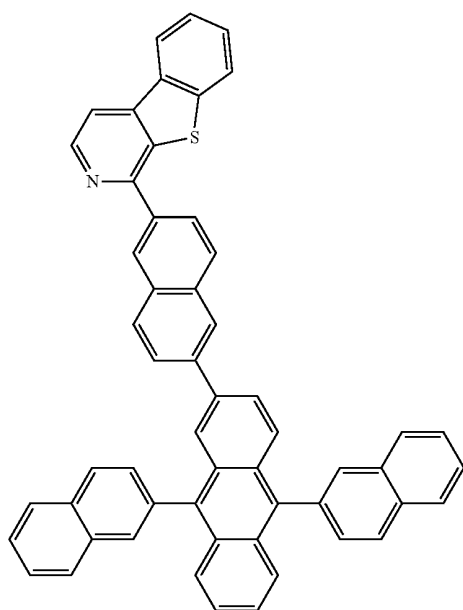


Compound 4



**47**

-continued



Compound 5

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Compound 6

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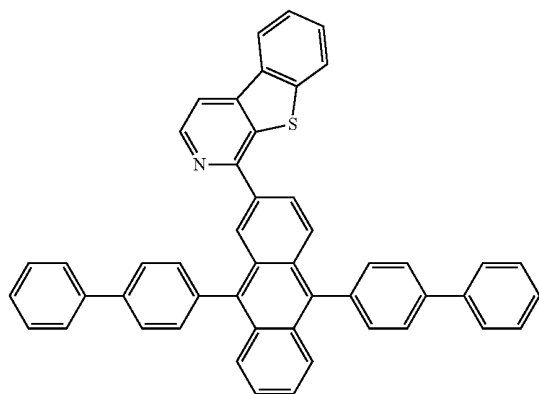
35

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Compound 7

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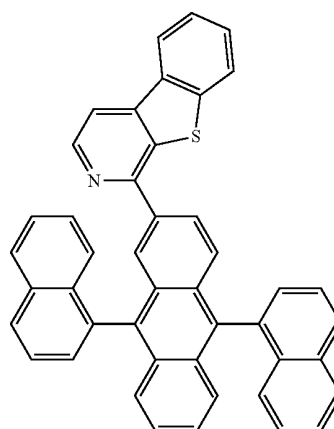
55

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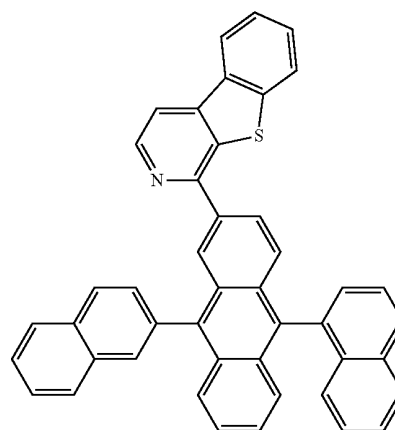
**48**

-continued

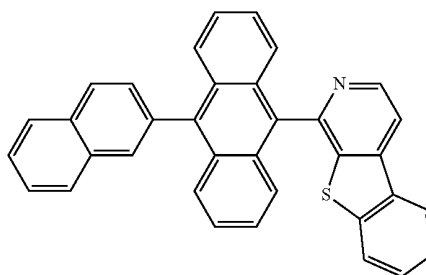


Compound 8

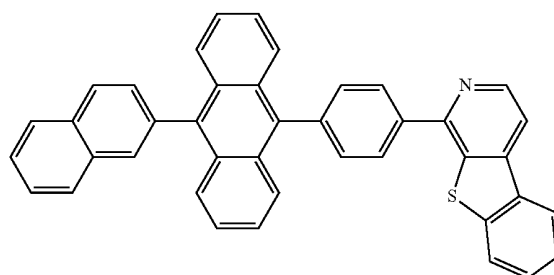
Compound 9



Compound 10



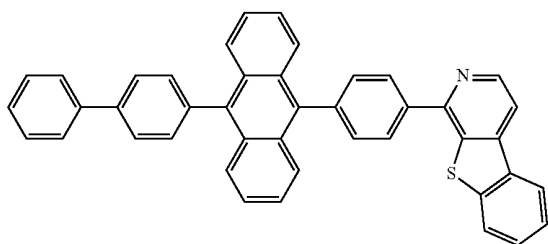
Compound 11



**49**

-continued

Compound 12

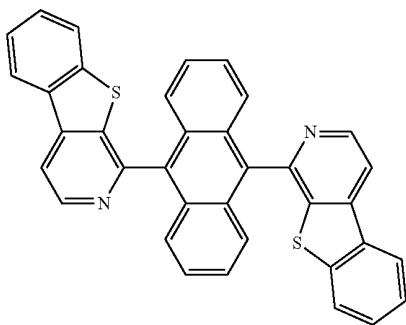


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Compound 13

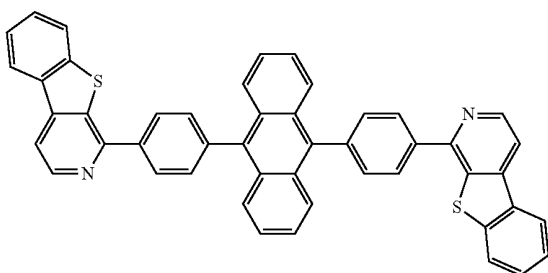


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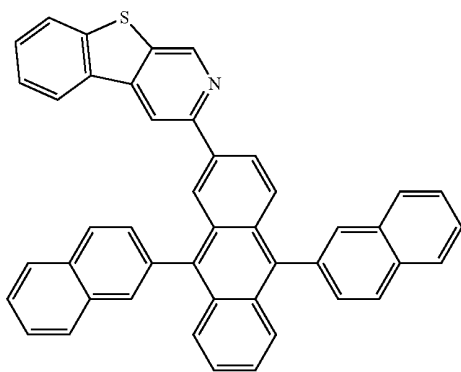
Compound 14



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Compound 15



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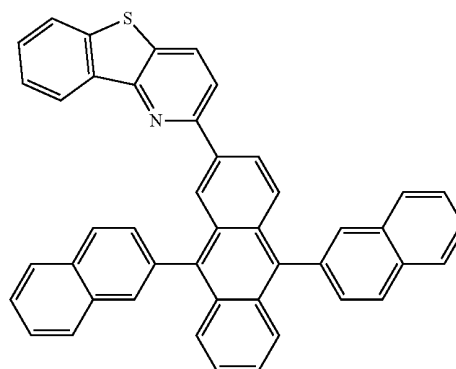
60

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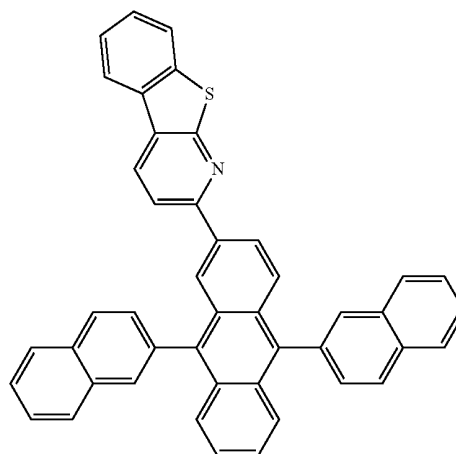
**50**

-continued

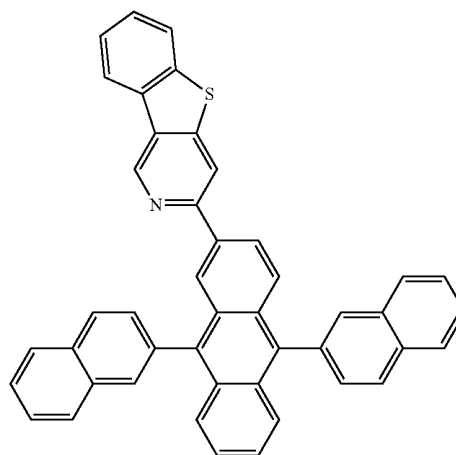
Compound 16



Compound 17



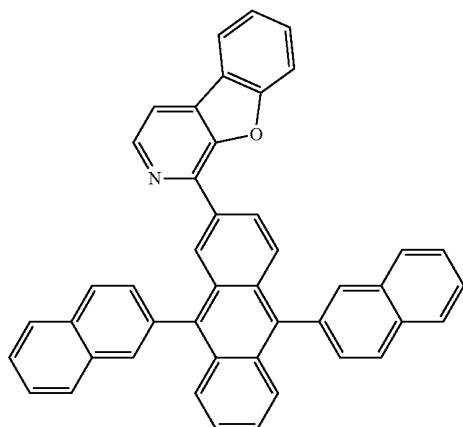
Compound 18



**51**

-continued

Compound 19



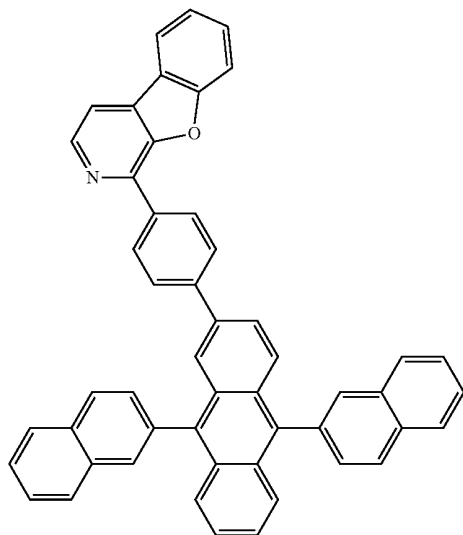
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Compound 20



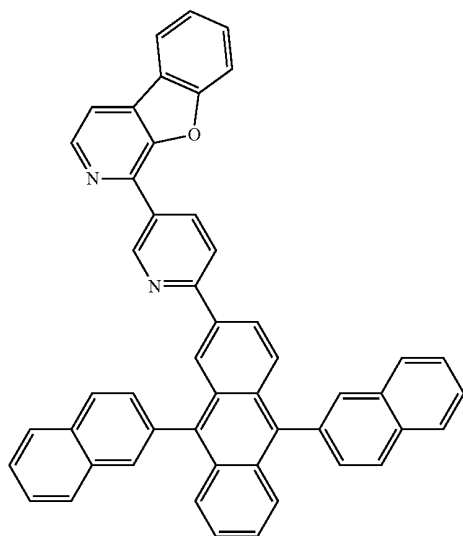
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Compound 21



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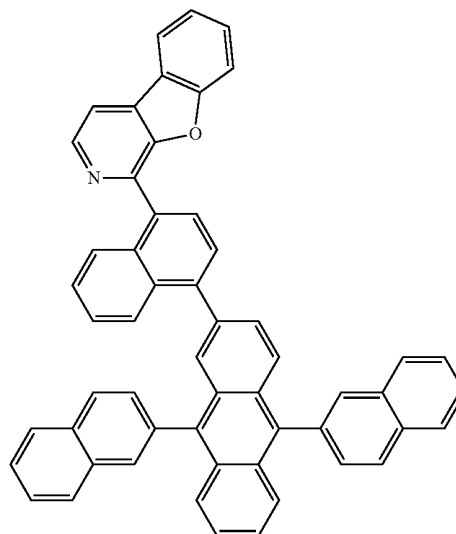
60

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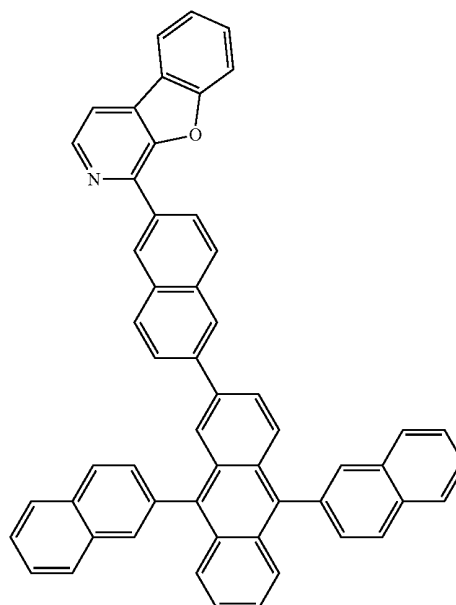
**52**

-continued

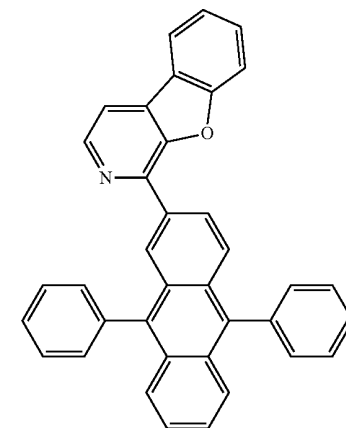
Compound 22



Compound 23



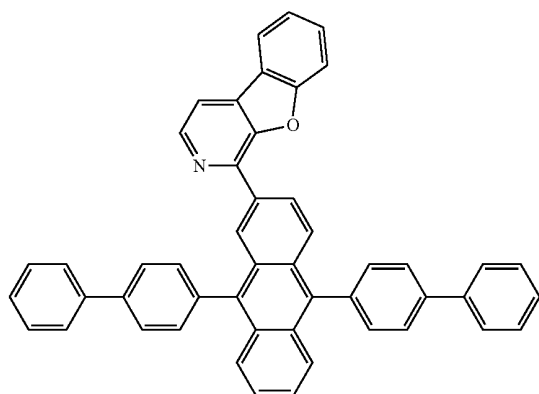
Compound 24



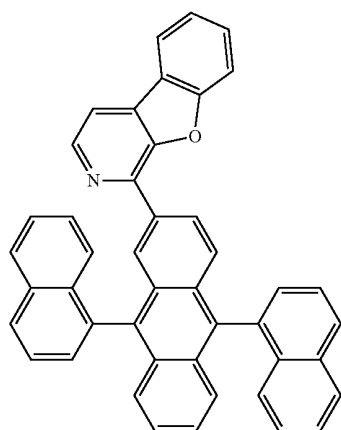


**53**

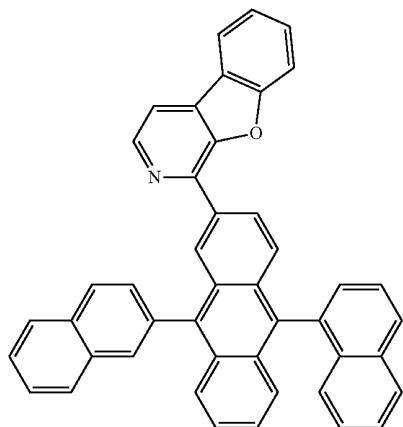
-continued



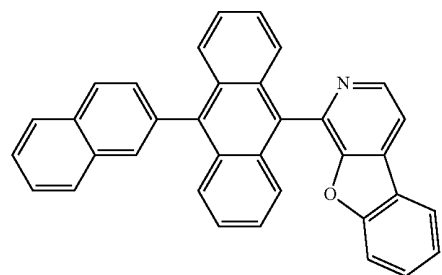
Compound 25



Compound 26



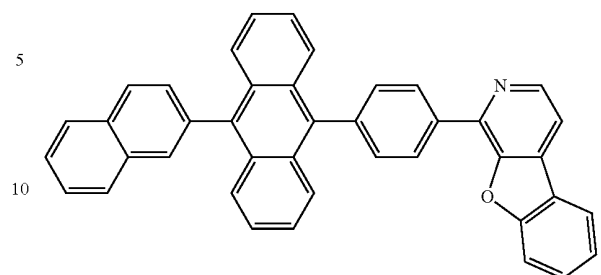
Compound 27



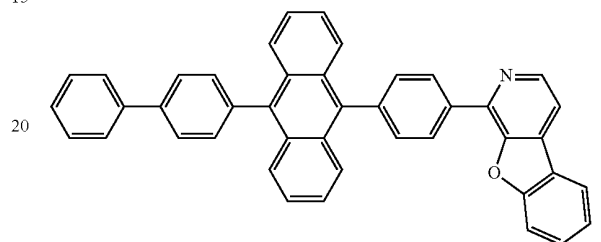
Compound 28

**54**

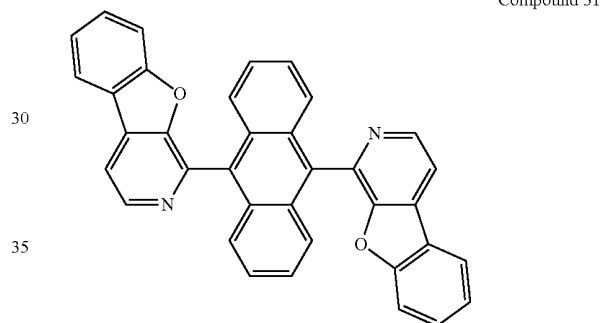
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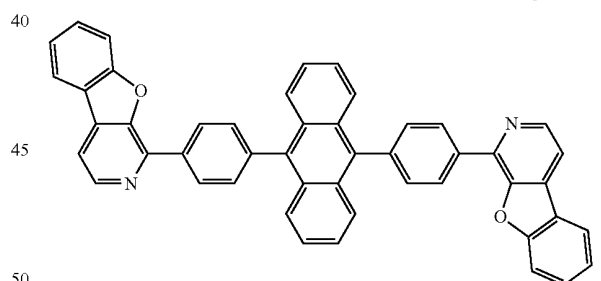
Compound 29



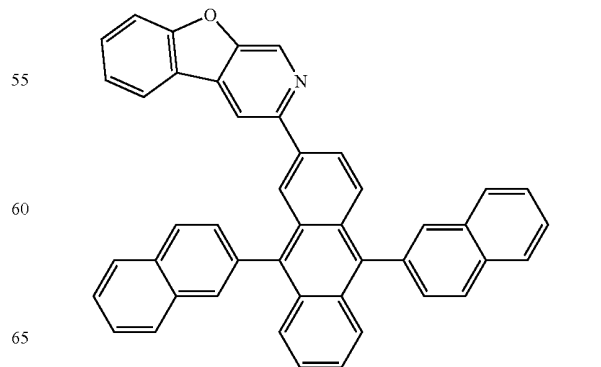
Compound 30



Compound 31



Compound 32

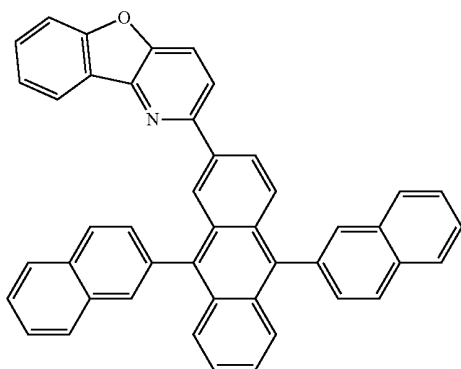


Compound 33

**55**

-continued

Compound 34



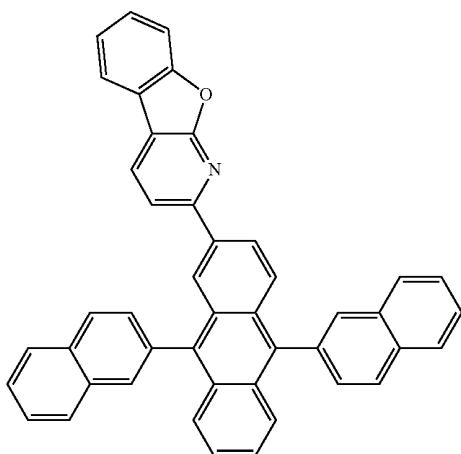
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Compound 35



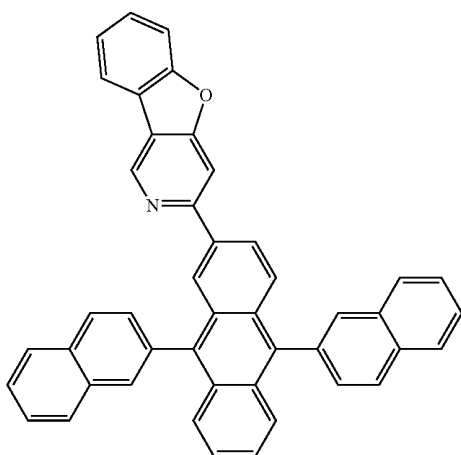
25

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Compound 36



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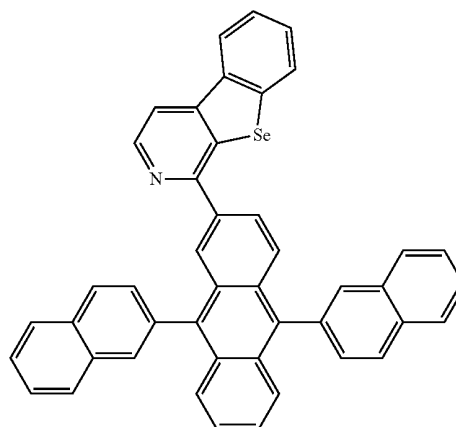
60

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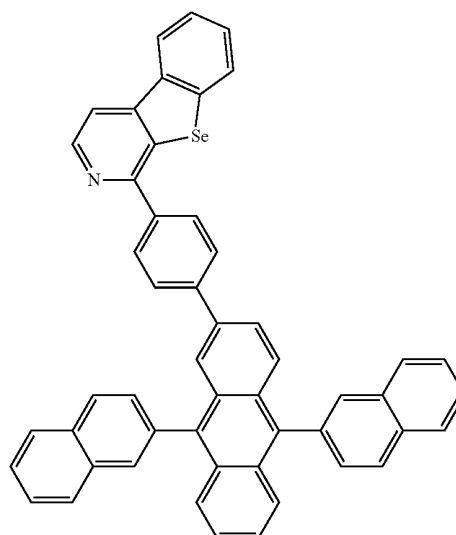
**56**

-continued

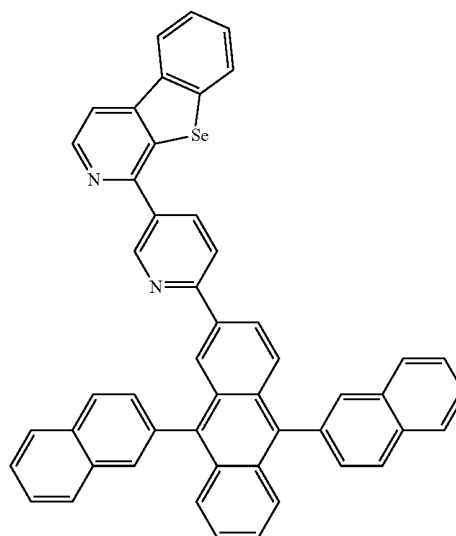
Compound 37



Compound 38

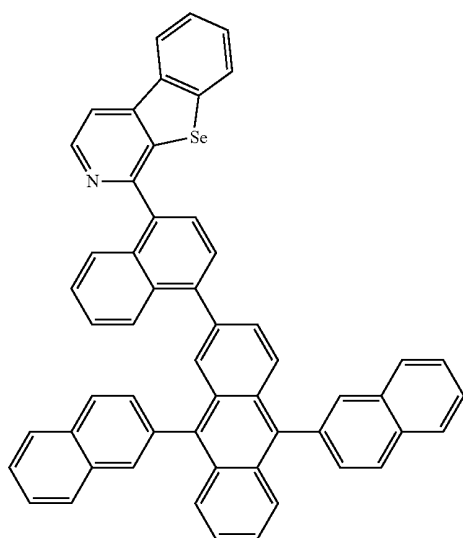


Compound 39



57

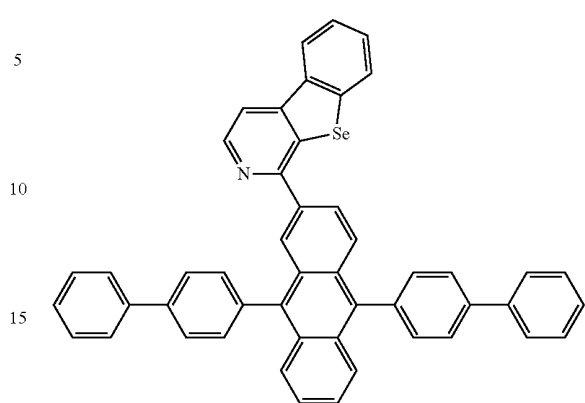
-continued



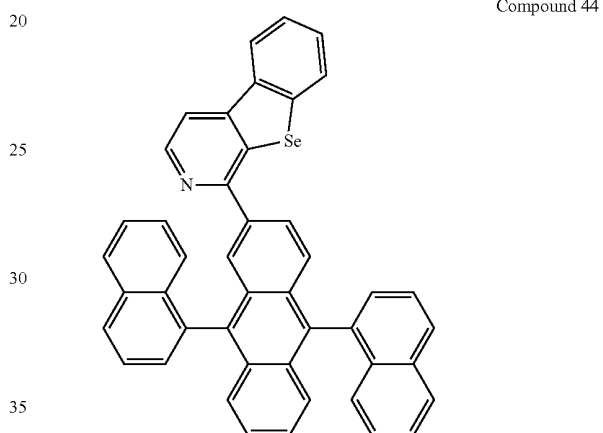
Compound 40

58

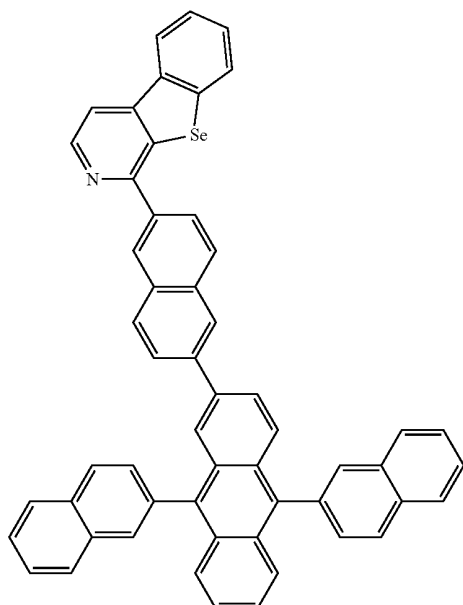
-continued



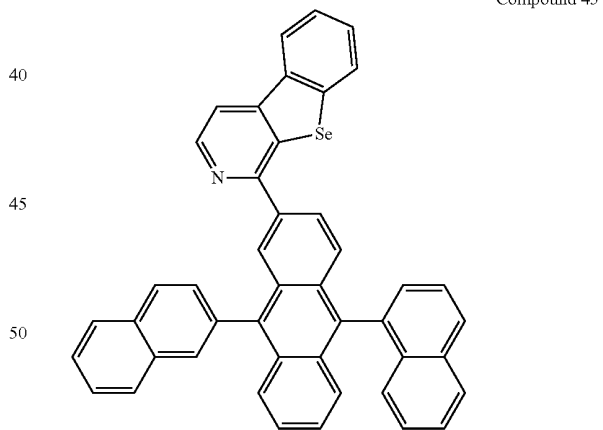
Compound 43



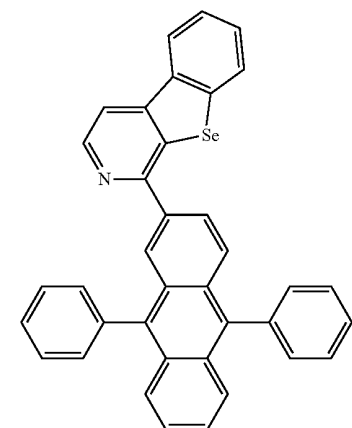
Compound 44



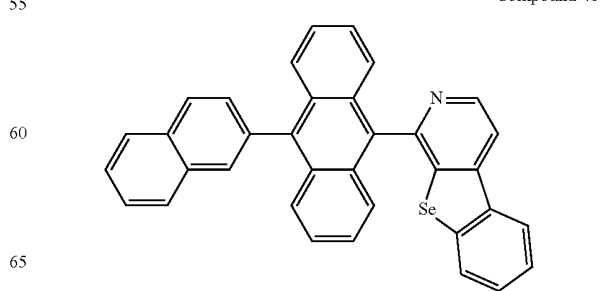
Compound 41



Compound 45



Compound 42

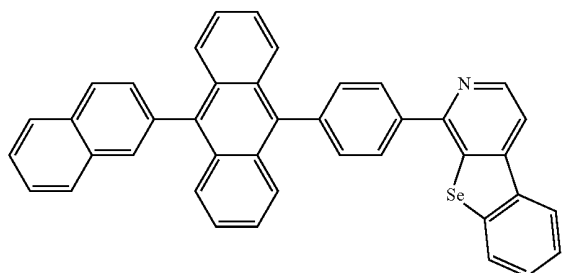


Compound 46

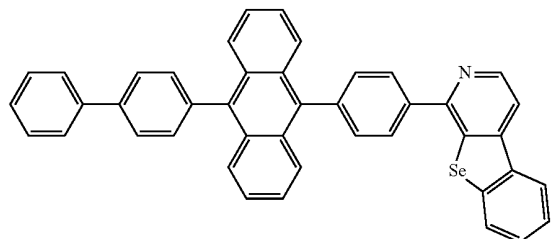
**59**

-continued

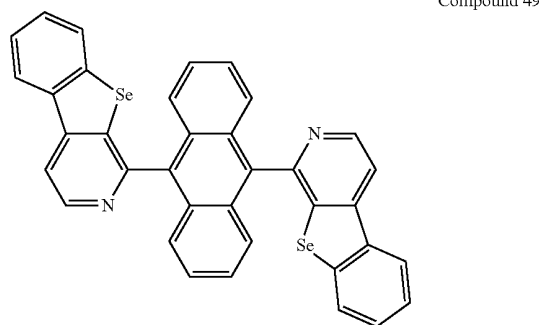
Compound 47



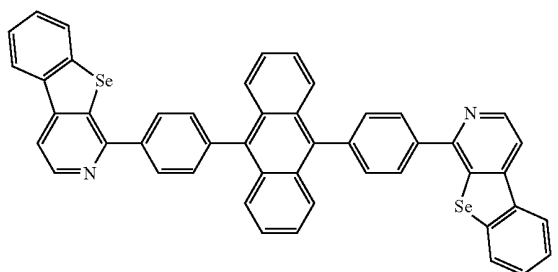
Compound 48



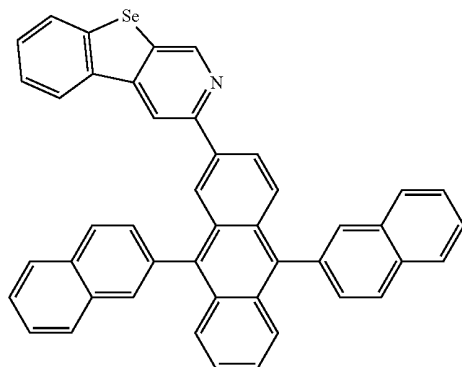
Compound 49



Compound 50

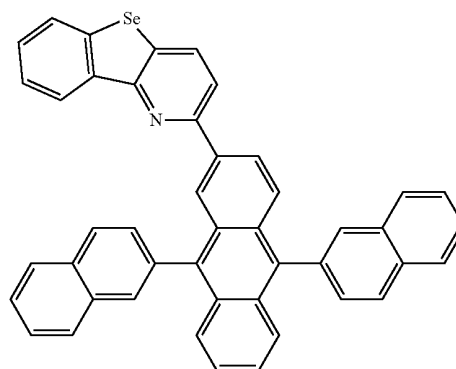


Compound 51

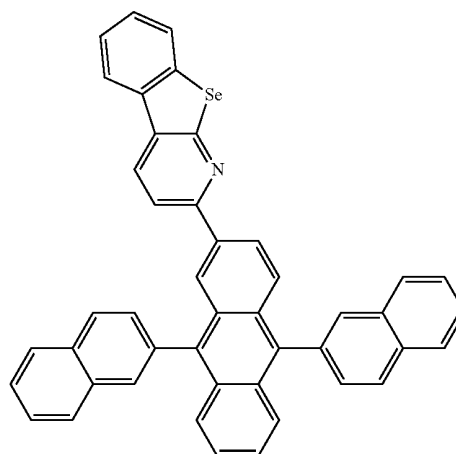
**60**

-continued

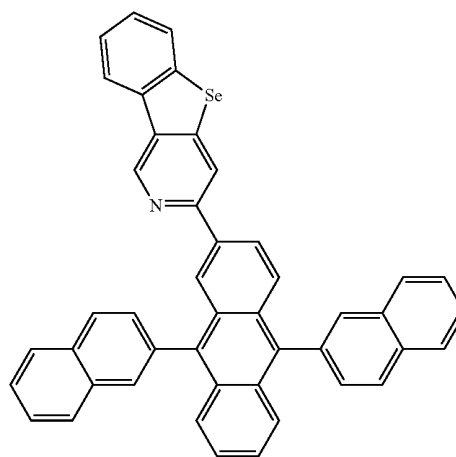
Compound 52



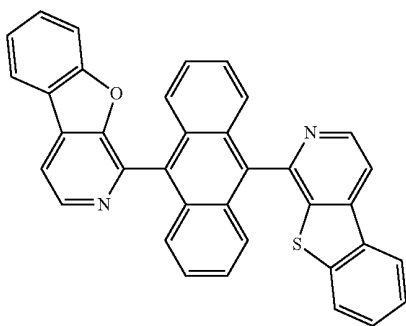
Compound 53



Compound 54



**61**  
-continued

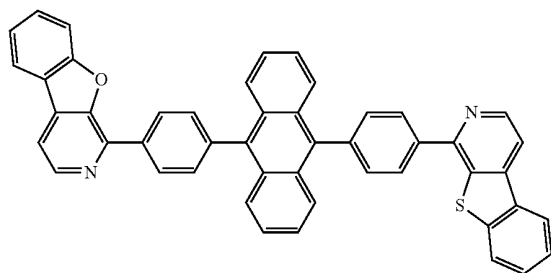


Compound 55

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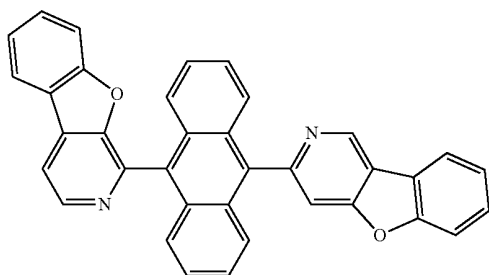
Compound 56

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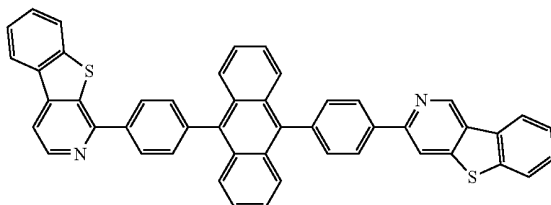
Compound 57



Compound 58

35

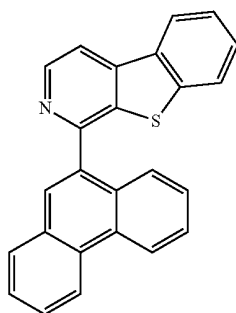
40



Compound 59

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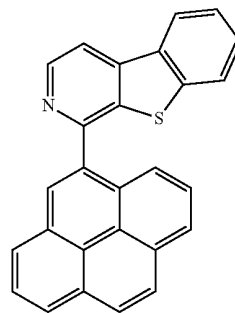


55

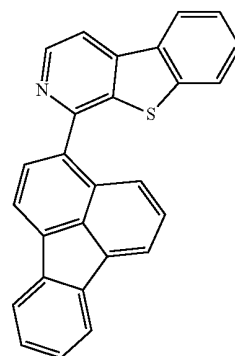
60

65

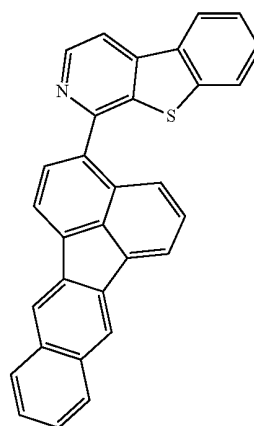
**62**  
-continued



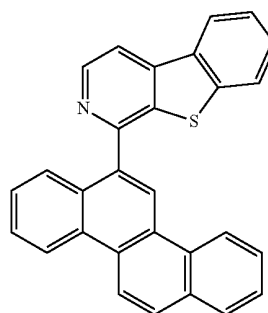
Compound 60



Compound 61



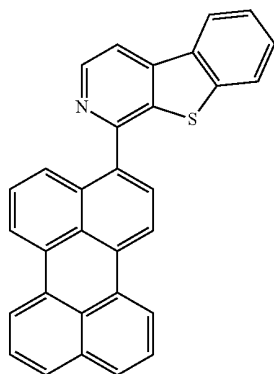
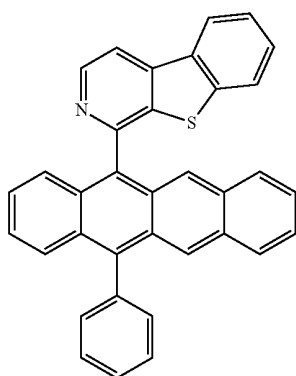
Compound 62



Compound 63

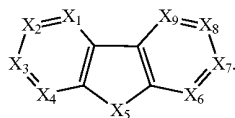
63

-continued



A first device comprising an organic light emitting device is also provided. The organic light emitting device comprises an anode, a cathode, and an organic layer that is disposed between the anode and the cathode. The organic layer comprises a compound having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$ .

Ar contains a condensed aromatic ring having at least three benzene rings and the condensed aromatic ring has a triplet energy lower than 440 nm. Ar is optionally further substituted. L is a single bond or a bivalent linking group. n is at least 1. i is an indexing variable that identifies n structures for  $\text{L}_i$  and  $\text{D}_i$  that may be the same or different for different values of i. Each  $\text{L}_i$  is independently a single bond or a bivalent linking group. Each  $\text{D}_i$  independently has the structure:



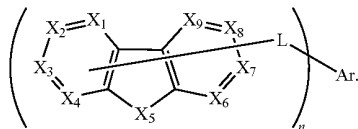
$\text{X}_5$  is O, S or Se. Each of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is independently selected from C(R) or N. At least one of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is N. Each R is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl. R is optionally bound to L.

The various specific aspects discussed above for compounds having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$  are also applicable to the compounds having formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$  when used in a first device. In particular, specific aspects of Ar, L, n, i,  $\text{L}_i$ ,  $\text{D}_i$ ,  $\text{X}_1$ - $\text{X}_9$ , R, R', R'', R<sub>1</sub>-R<sub>6</sub>, Formula I, Formula II, Formula III, Formula IV, Formula V and Formula VI of the compounds

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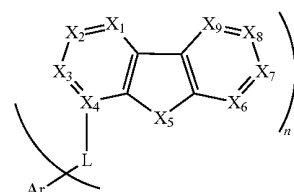
having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$ , as discussed above, are also applicable to a compound having the formula  $\text{Ar}(\text{L}_i\text{D}_i)_n$  that is used in the first device.

In one aspect, the compound has the formula:

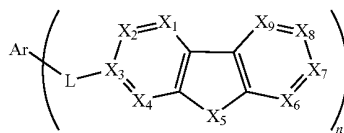


Formula I

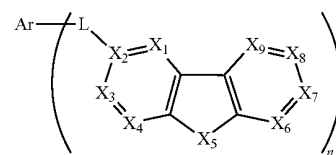
In another aspect, the compound has a formula selected from the group consisting of:



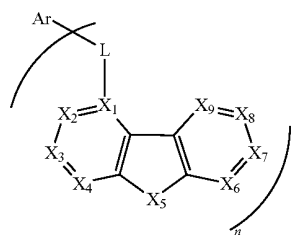
Formula II



Formula III

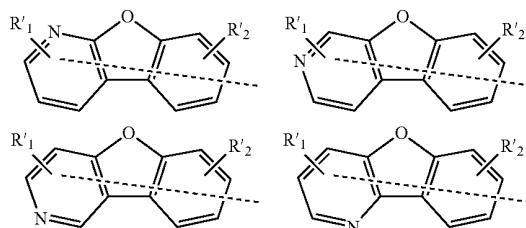


Formula IV



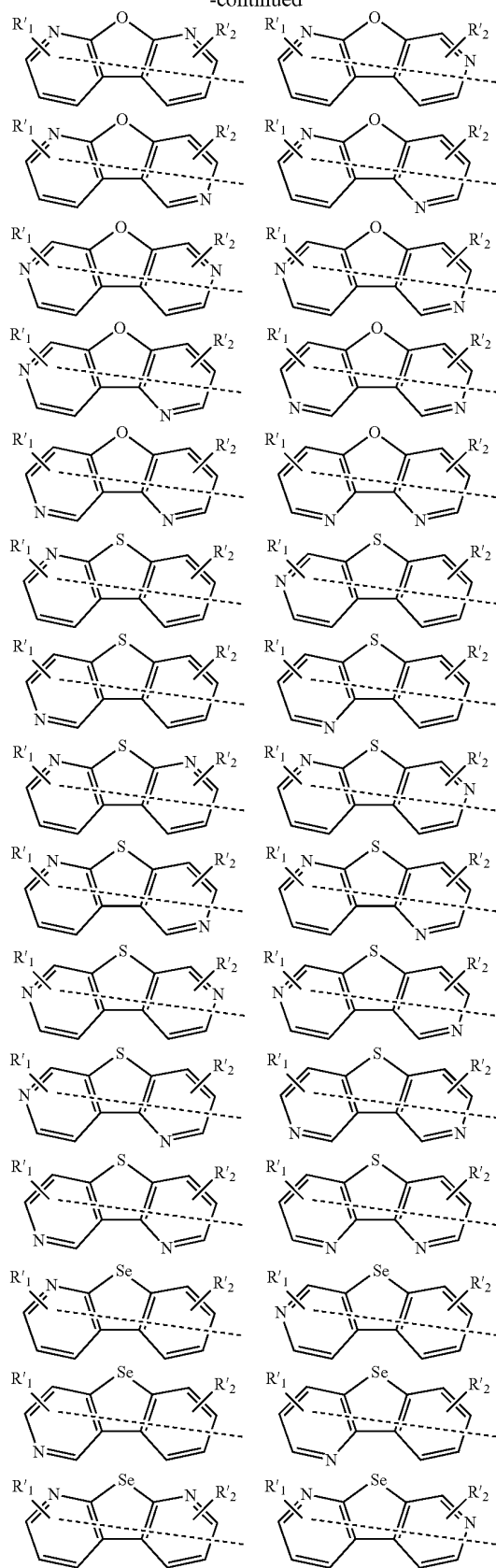
Formula V

In one aspect, each  $\text{D}_i$  is independently selected from the group consisting of:



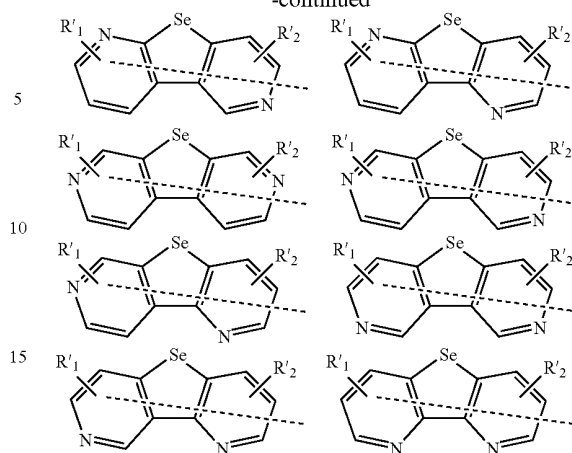
65

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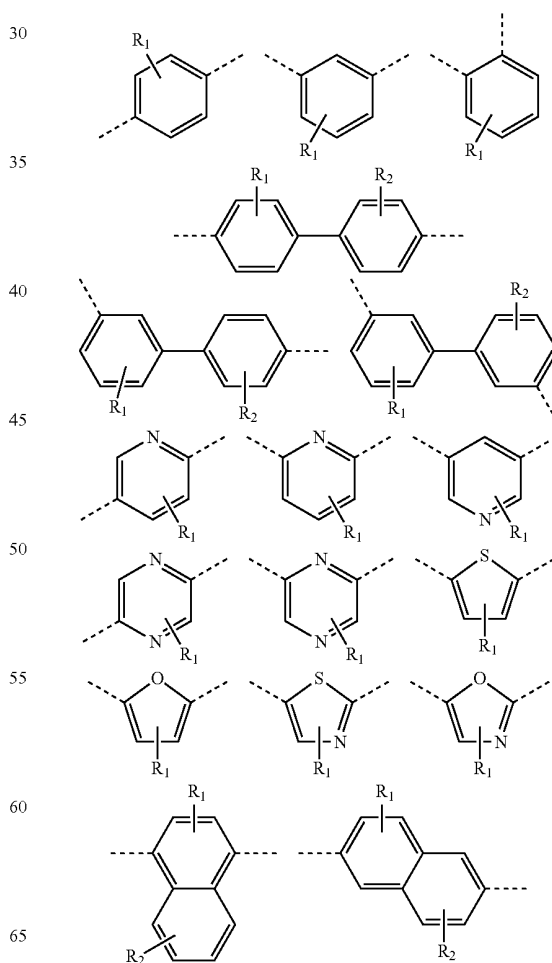
66

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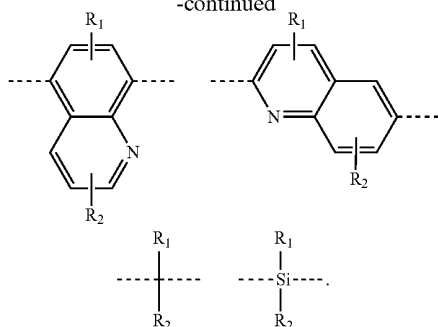
$R'_1$  and  $R'_2$  may represent mono, di, tri, or tetra substitutions.  $R'_1$  and  $R'_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect, L is a single bond. In another aspect, each  $L_i$  is independently selected from the group consisting of:



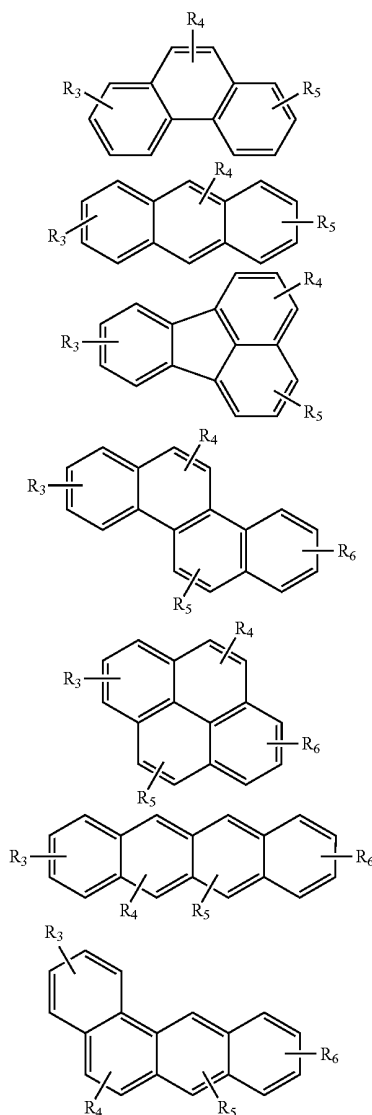
67

-continued



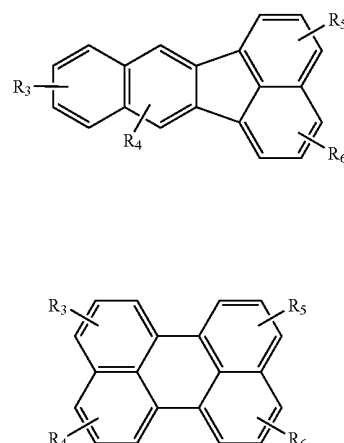
$R_1$  and  $R_2$  may represent mono, di, tri, or tetra substitutions.  $R_1$  and  $R_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect, Ar is selected from the group consisting of:



68

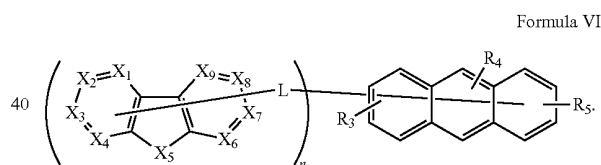
-continued



$R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  may represent mono, di, tri, or tetra substitutions.  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

In one aspect,  $n$  is 1. In another aspect,  $n$  is greater than 1 and each  $D_i$  has the same structure. In yet another aspect,  $n$  is greater than 1 and at least two  $D_i$  have different structures. In a further aspect,  $n$  is 2.

Preferably, the compound has the formula:



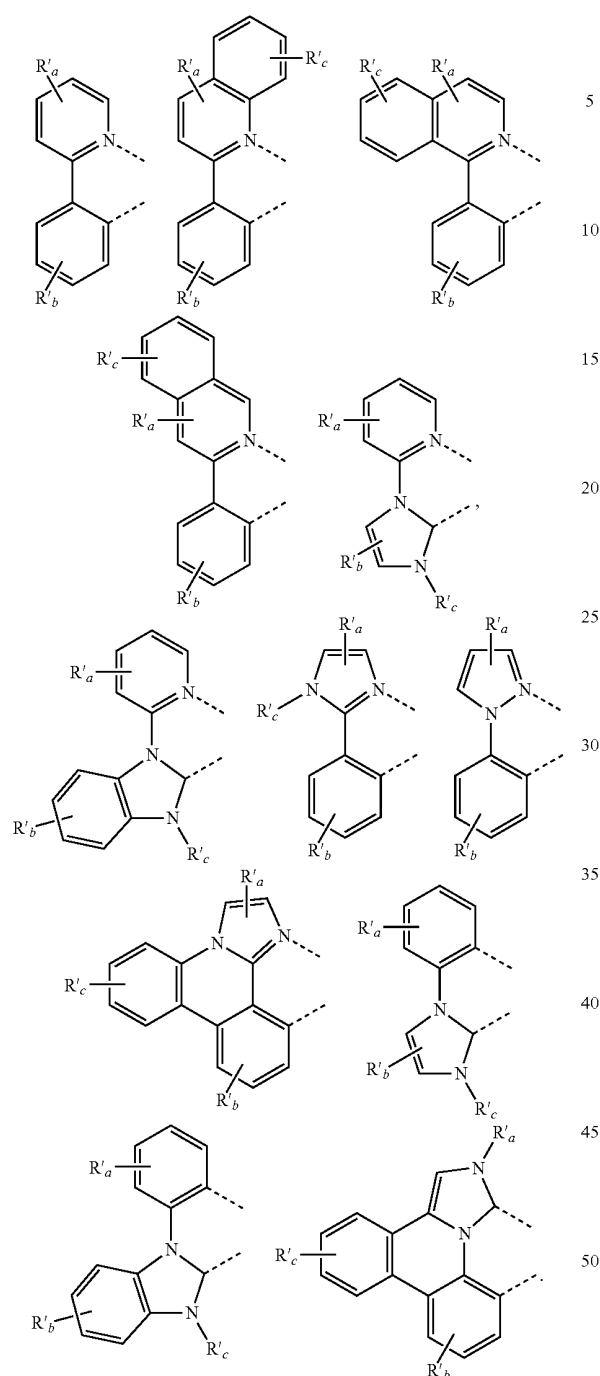
$R_3$ ,  $R_4$ , and  $R_5$  may represent mono, di, tri, or tetra substitutions.  $R_3$ ,  $R_4$ , and  $R_5$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

Specific examples of devices comprising the compounds disclosed herein are provided. In one aspect, the compound used in the first device is selected from the group consisting of Compound 1-Compound 65.

In one aspect, the organic layer is a non-emissive layer and the compound is a non-emissive compound. In another aspect, the organic layer is an electron transport layer and the compound is an electron transport material. In yet another aspect, the electron transporting layer is doped with an n-type conductivity dopant. In one aspect, the n-type conductivity dopant is a compound containing Li, Na, K, Rb, or Cs. Preferably, the n-type conductivity dopant is selected from the group consisting of LiF, CsF, NaCl, KBr, and LiQ.

In another aspect, the organic layer further comprises an emissive compound that is a transition metal complex having at least one ligand selected from the group consisting of:





Each of  $R'_a$ ,  $R'_b$  and  $R'_c$  may represent mono, di, tri, or tetra substituents. Each of  $R'_a$ ,  $R'_b$  and  $R'_c$  are independently selected from a group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, or heteroaryl. Two adjacent substituents may form into a ring.

In one aspect, the first device is a consumer product. In another aspect, the first device is an organic light emitting device.

#### Combination with Other Materials

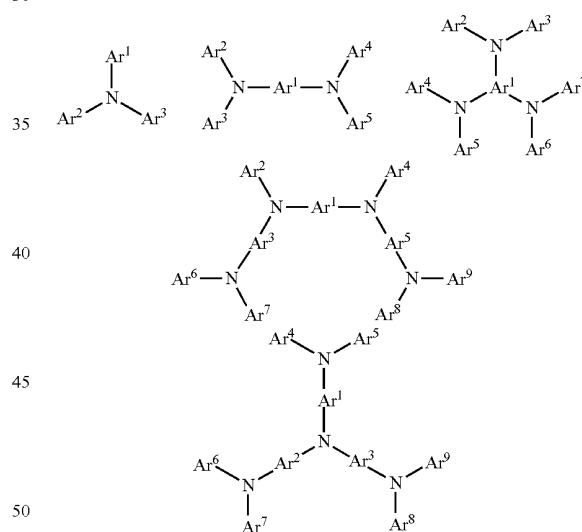
The materials described herein as useful for a particular layer in an organic light emitting device may be used in

combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

#### HIL/HTL:

A hole injecting/transporting material to be used in embodiments of the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but are not limited to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as  $\text{MoO}_3$ ; a p-type semiconducting organic compound, such as 1, 4, 5, 8, 9, 12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

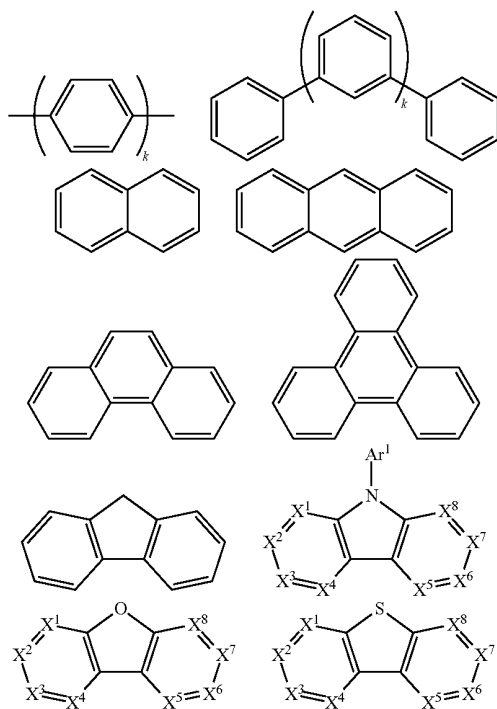
Examples of aromatic amine derivatives used in HIL or HTL include, but are not limited to the following general structures:



Each of  $\text{Ar}^1$  to  $\text{Ar}^9$  is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyrindine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene,

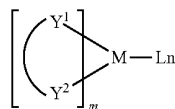
acridine, phenazine, phenothiazine, phenoxazine, benzofuro-pyridine, furodipyridine, benzothienopyridine, thienodipyri-dine, benzoselenophenopyridine, and selenophenodipyri-dine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consist-ing of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

In one aspect, Ar<sup>1</sup> to Ar<sup>9</sup> is independently selected from the group consisting of:



k is an integer from 1 to 20; X<sup>1</sup> to X<sup>8</sup> is CH or N; Ar<sup>1</sup> has the same group defined above.

Examples of metal complexes used in HIL or HTL include, but are not limited to the following general formula:



M is a metal, having an atomic weight greater than 40; (Y<sup>1</sup>-Y<sup>2</sup>) is a bidentate ligand, Y<sup>1</sup> and Y<sup>2</sup> are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

In one aspect, (Y<sup>1</sup>-Y<sup>2</sup>) is a 2-phenylpyridine derivative.

In another aspect, (Y<sup>1</sup>-Y<sup>2</sup>) is a carbene ligand.

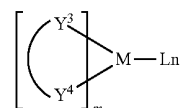
In another aspect, M is selected from Ir, Pt, Os, and Zn.

In a further aspect, the metal complex has a smallest oxi-dation potential in solution vs. Fc<sup>+</sup>/Fc couple less than about 0.6 V.

Host:

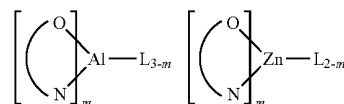
The light emitting layer of the organic EL device in some embodiments of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant.

Examples of metal complexes used as hosts are preferred to have the following general formula:



M is a metal; (Y<sup>3</sup>-Y<sup>4</sup>) is a bidentate ligand, Y<sup>3</sup> and Y<sup>4</sup> are independently selected from C, N, O, P, and S; L is an ancil-lary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

In one aspect, the metal complexes are:



(O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

In another aspect, M is selected from Ir and Pt.

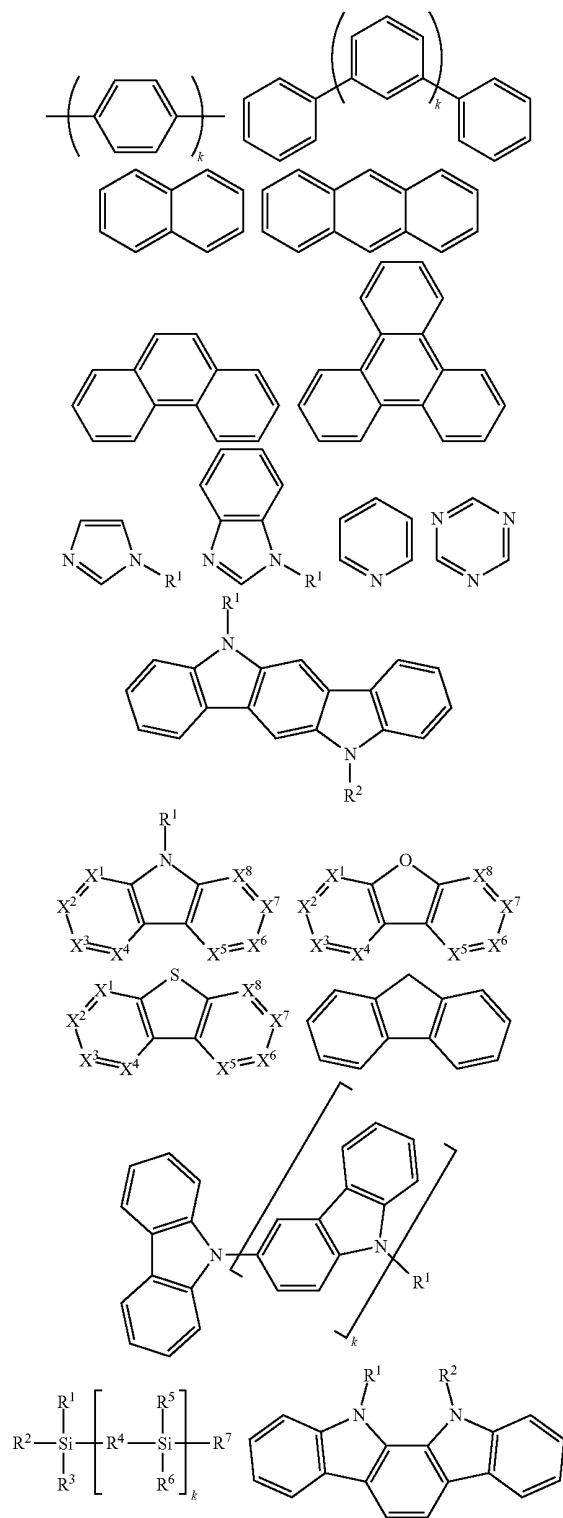
In a further aspect, (Y<sup>3</sup>-Y<sup>4</sup>) is a carbene ligand.

Examples of organic compounds used as hosts are selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consist-ing of aromatic heterocyclic compounds such as diben-zothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyri-dine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadia-zole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiaz-ine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, iso-quinoline, cinnoline, quinazoline, quinoxaline, naphthyri-dine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuro-pyridine, furodipyri-dine, benzothienopyridine, thienodipyridine, benzosele-nophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substi-tuted by a substituent selected from the group consisting of

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hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

In one aspect, the host compound contains at least one of the following groups in the molecule:



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$R^1$  to  $R^7$  is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

$k$  is an integer from 0 to 20.

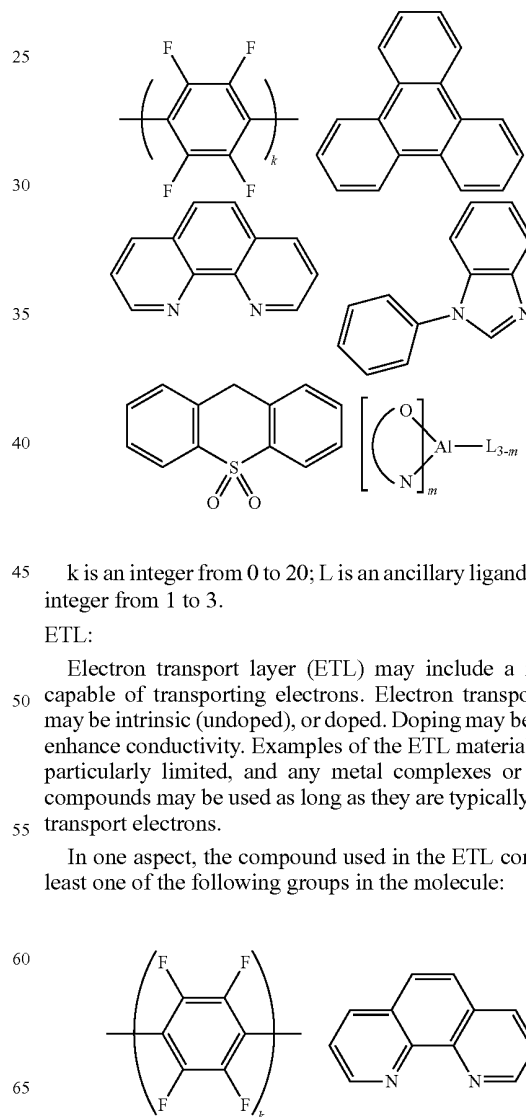
$X^1$  to  $X^8$  is selected from CH or N.

HBL:

A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED.

In one aspect, the compound used in the HBL contains the same molecule used as host described above.

In another aspect, the compound used in the HBL contains at least one of the following groups in the molecule:

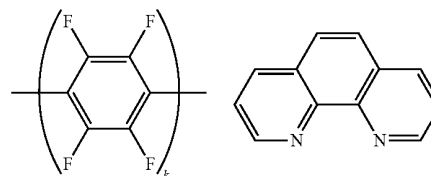


$k$  is an integer from 0 to 20;  $L$  is an ancillary ligand,  $m$  is an integer from 1 to 3.

ETL:

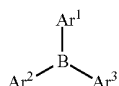
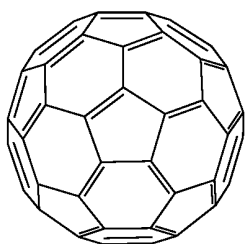
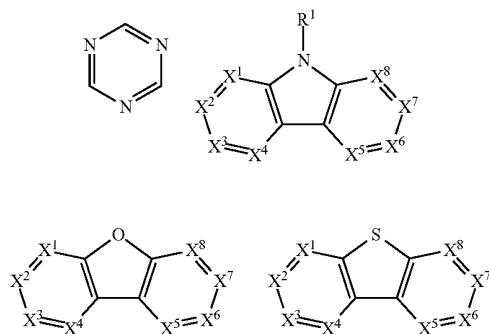
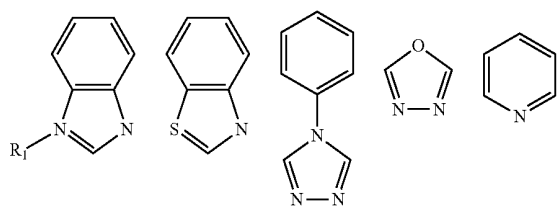
Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

In one aspect, the compound used in the ETL contains at least one of the following groups in the molecule:



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-continued



$R^1$  is selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, het-

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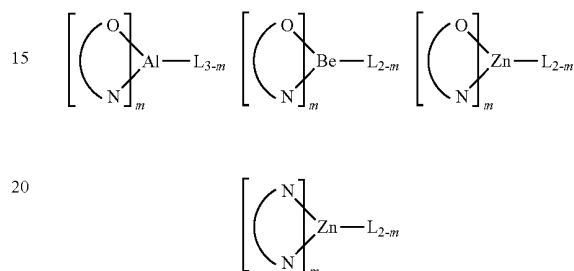
eroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

$Ar^1$  to  $Ar^3$  has the similar definition as Ar's mentioned above.

$k$  is an integer from 0 to 20.

$X^1$  to  $X^8$  is selected from CH or N.

In another aspect, the metal complexes used in the ETL contain, but are not limited to, the following general formula:



(O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L is an ancillary ligand;  $m$  is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

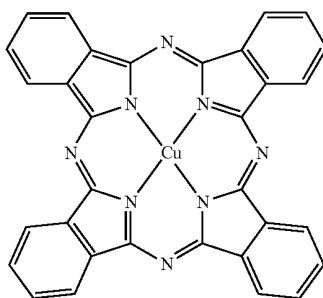
In any of the above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated.

In addition to and/or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exciton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 2 below. Table 2 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 2

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		

Phthalocyanine  
and  
porphyrin  
compounds



Appl. Phys.  
Lett. 69,  
2160 (1996)

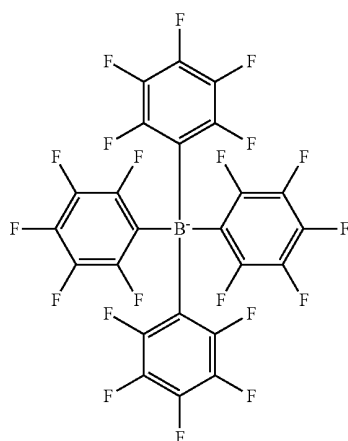
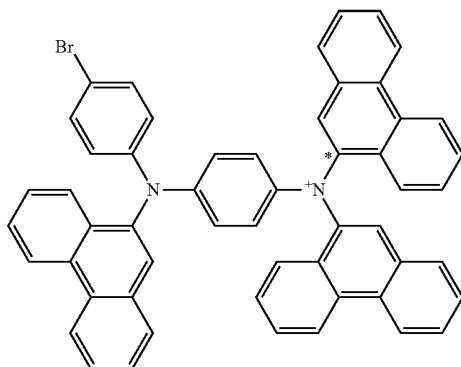
TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Starburst triarylamine		J. Lumin. 72-74, 985 (1997)
CF <sub>x</sub> Fluoro- hydrocarbon polymer		Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and siliane SAMs		U.S. Pat. No. 20030162053
Triarylamine or polythiophene polymers with conductivity dopants		EA01725079A1

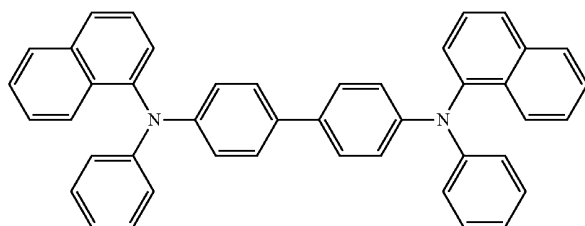
TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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and

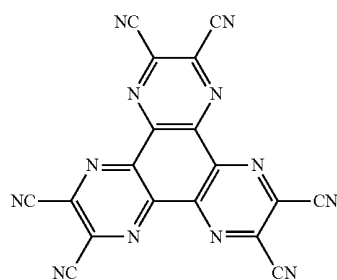


Arylamines  
complexed  
with metal  
oxides such  
as molybdenum  
and tungsten  
oxides

+ MoO<sub>x</sub>

SID Symposium  
Digest, 37, 923  
(2006)  
WO2009018009

Semiconducting  
organic  
complexes



U.S. Pat. No.  
20020158242

TABLE 2-continued

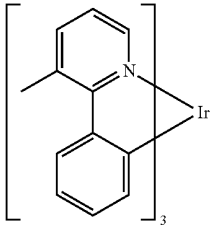
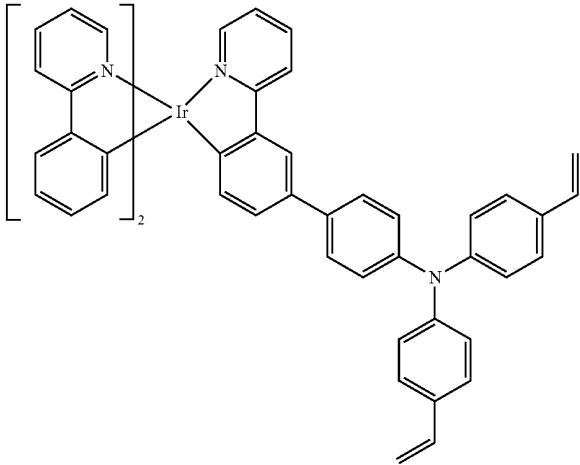
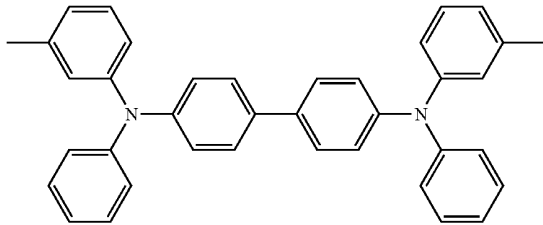
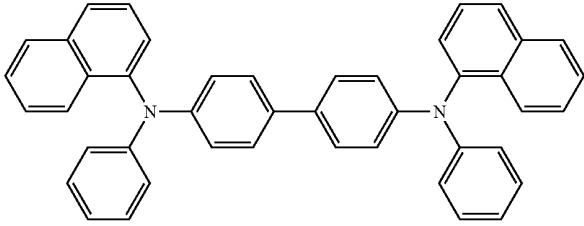
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal organometallic complexes		U.S. Pat. No. 20060240279
Cross-linkable compounds		U.S. Pat. No. 20080220265
Hole transporting materials		
Triarylamines (e.g., TPD, $\alpha$ -NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5061569

TABLE 2-continued

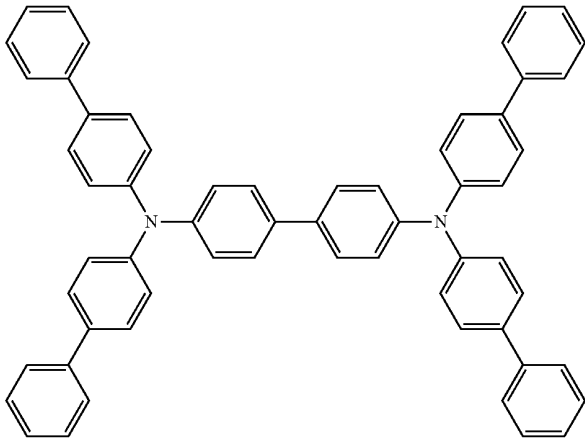
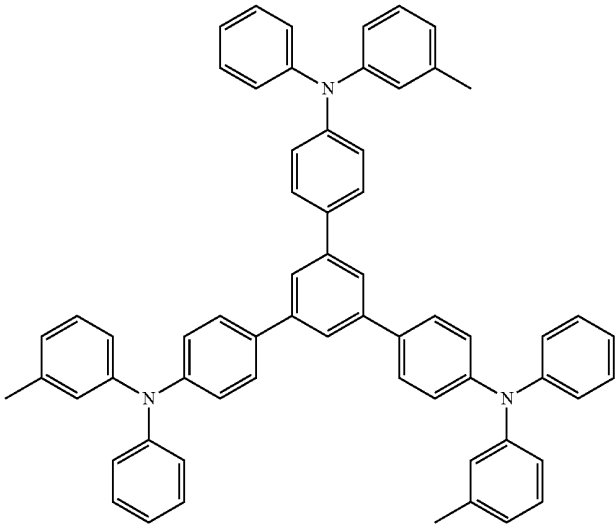
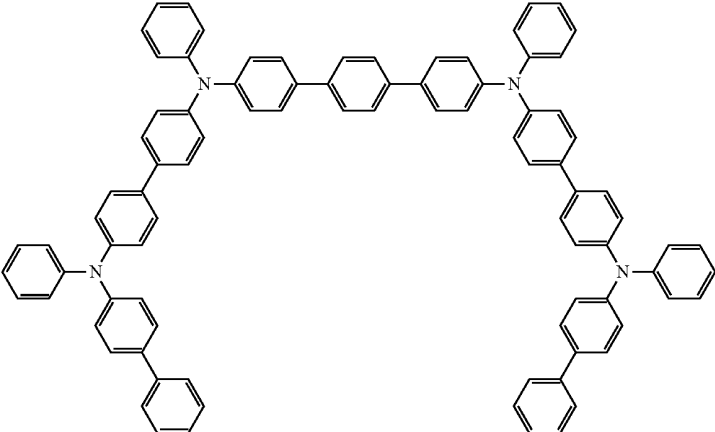
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		EP650955
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)



TABLE 2-continued

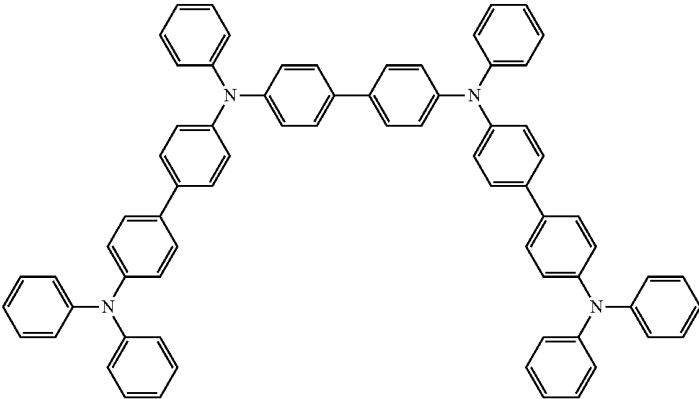
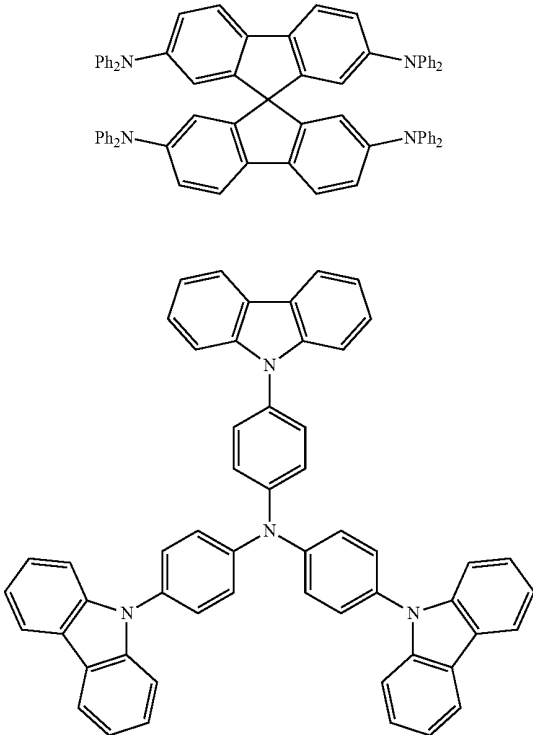
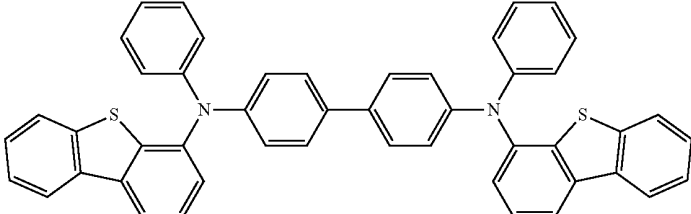
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine on spirofluorene core		Appl. Phys. Lett. 90, 183503 (2007)
Arylamine carbazole compounds		Synth. Met. 91, 209 (1997)
Triarylamine with (di)benzo- thiophene/ (di)benzofuran		U.S. Pat. No. 20070278938, U.S. Pat. No. 20080106190

TABLE 2-continued

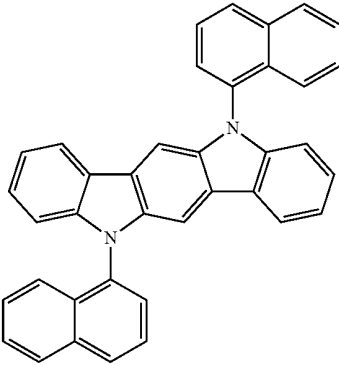
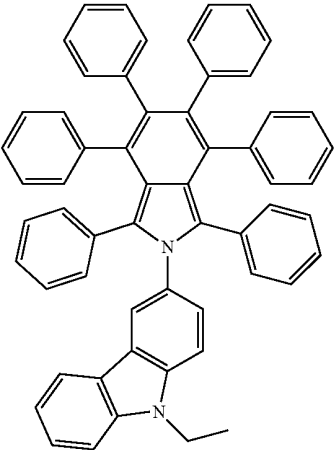
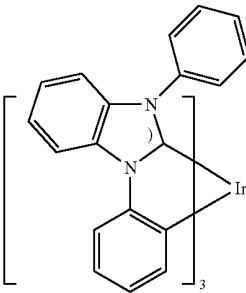
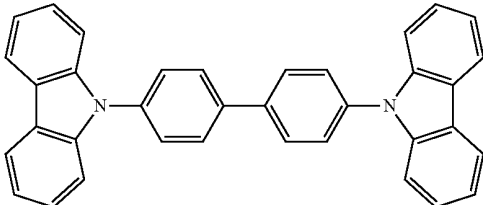
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		U.S. Pat. No. 20080018221
Phosphorescent OLED host materials		
Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 2-continued

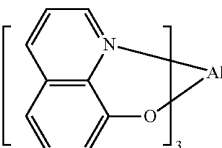
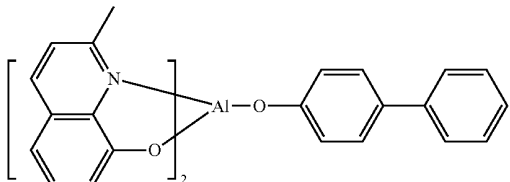
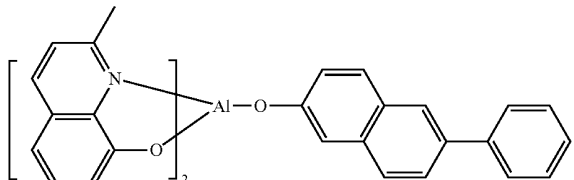
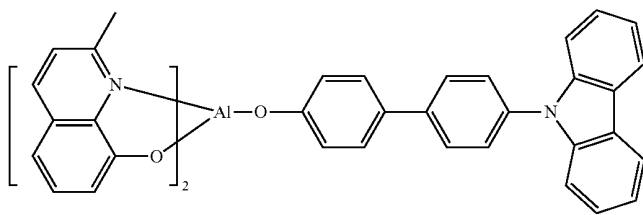
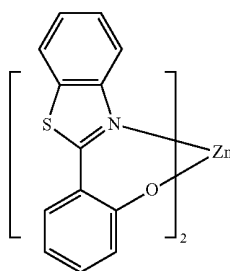
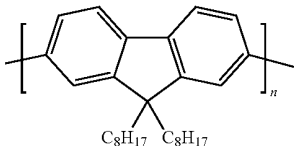
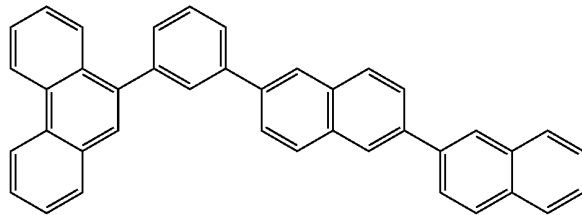
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal 8-hydroxyquinolates (e.g., Alq <sub>3</sub> , BAlq)		Nature 395, 151 (1998)
		U.S. Pat. No. 20060202194
		WO2005014551
		WO2006072002
Metal phenoxy-benzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, U.S. Pat. No. 20090045731, U.S. Pat. No. 20090045730, WO2009008311, U.S. Pat. No. 20090008605, U.S. Pat. No. 20090009065

TABLE 2-continued

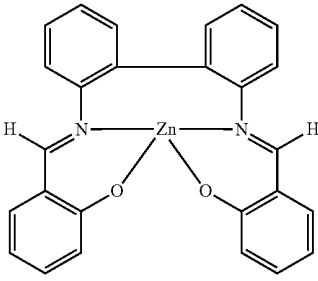
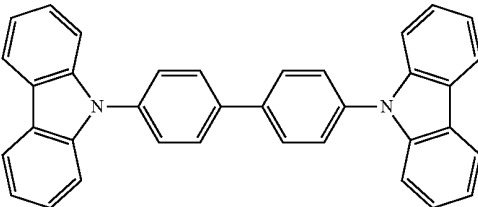
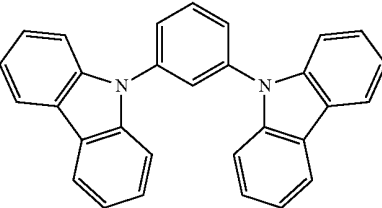
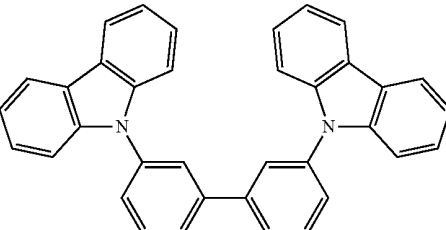
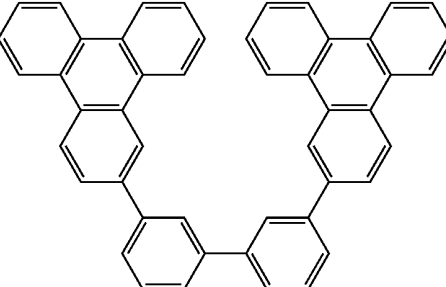
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Zinc complexes		WO2009062578
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		U.S. Pat. No. 20030175553
		WO2001039234
Aryltriphenylene compounds		U.S. Pat. No. 20060280965

TABLE 2-continued

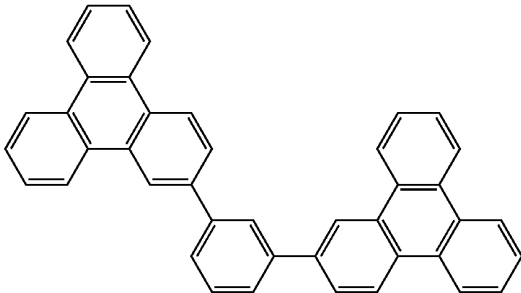
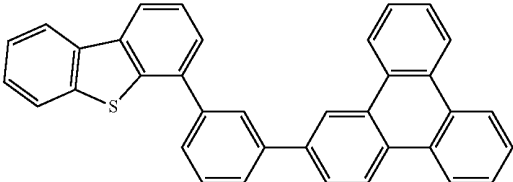
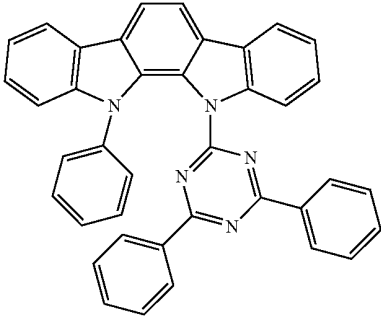
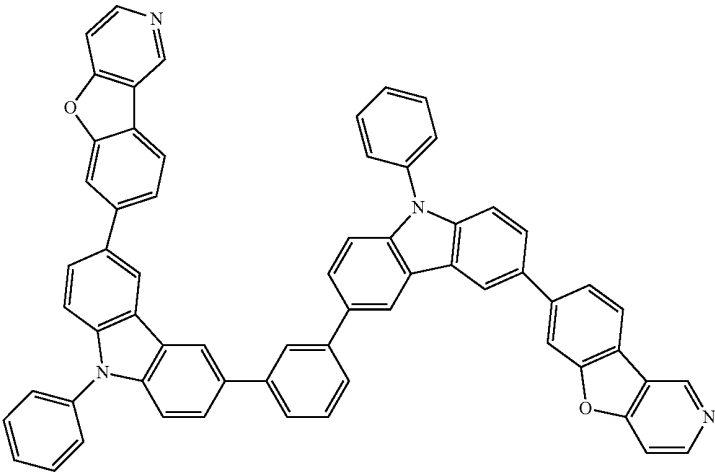
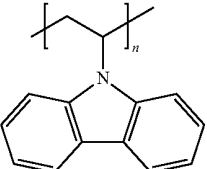
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Donor acceptor type molecules		U.S. Pat. No. 20060280965
		WO2009021126
		WO2008056746
Aza-carbazole/ DBT/DBF		JP2008074939
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)

TABLE 2-continued

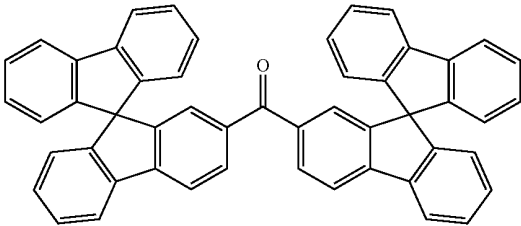
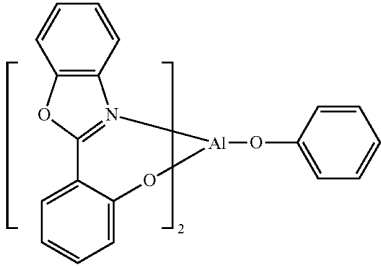
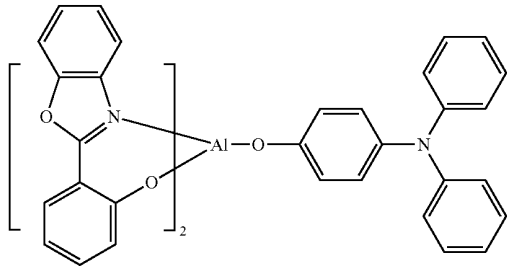
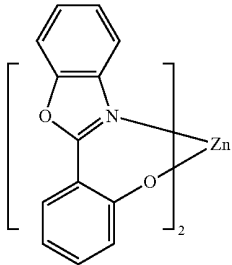
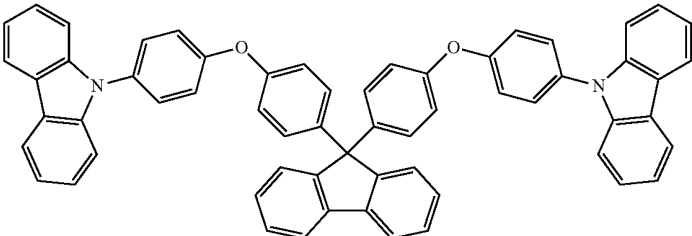
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Spirofluorene compounds		WO2004093207
Metal phenoxy-benzoxazole compounds		WO2005089025
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocabazoles		JP2007254297
		WO2007063796
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822

TABLE 2-continued

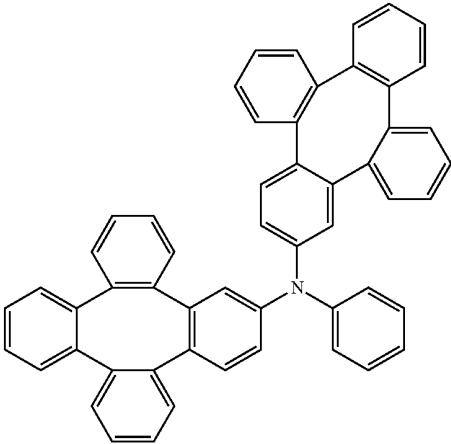
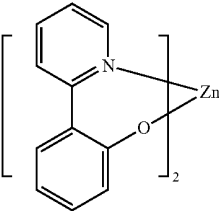
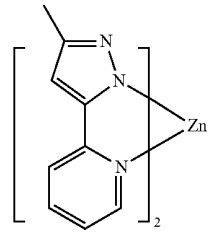
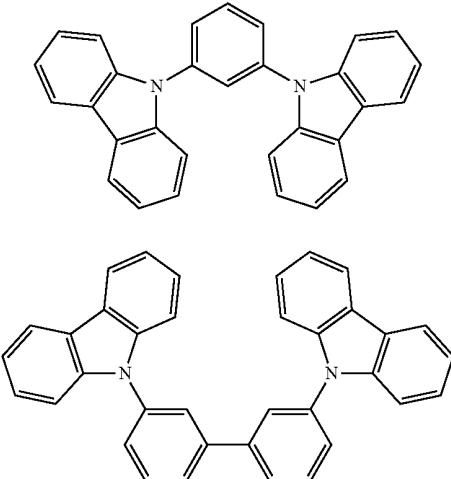
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		U.S. Pat. No. 20050112407
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N-N ligands)		U.S. Pat. No. 20040137268, U.S. Pat. No. 20040137267
Blue hosts		
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		U.S. Pat. No. 20070190359



TABLE 2-continued

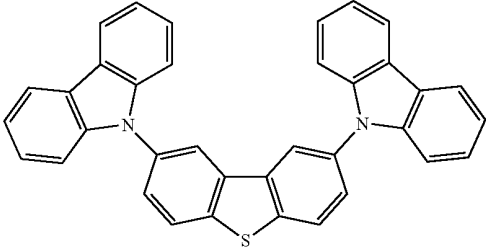
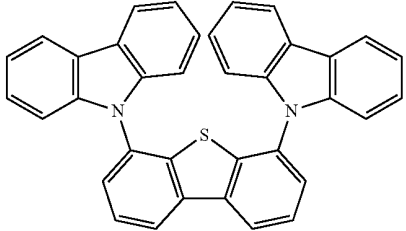
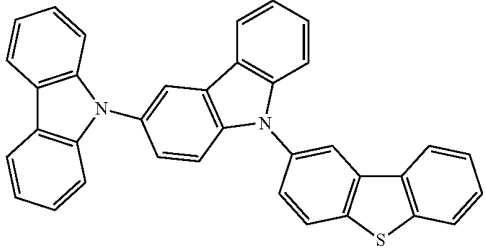
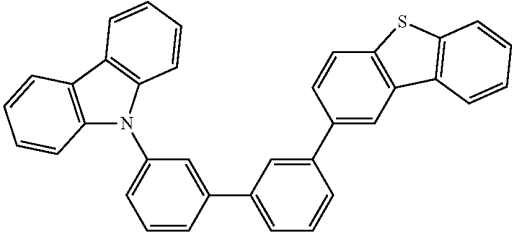
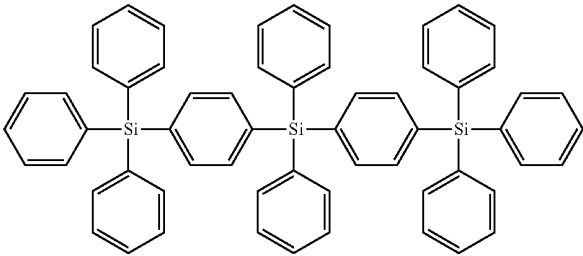
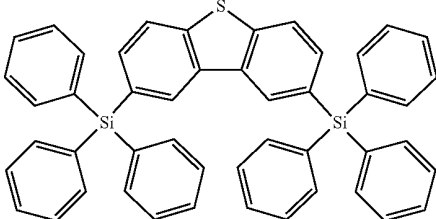
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzo- thiophene/ Dibenzofuran- carbazole compounds		WO2006114966, U.S. Pat. No. 20090167162
		U.S. Pat. No. 20090167162
		WO2009086028
		U.S. Pat. No. 20090030202, U.S. Pat. No. 20090017330
Silicon aryl compounds		U.S. Pat. No. 20050238919
		WO2009003898

TABLE 2-continued

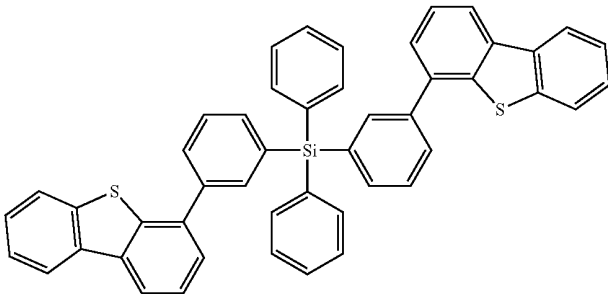
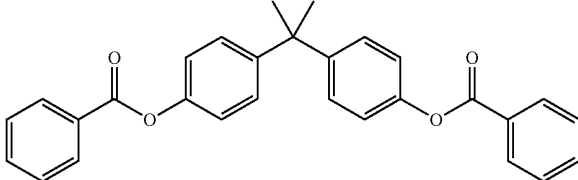
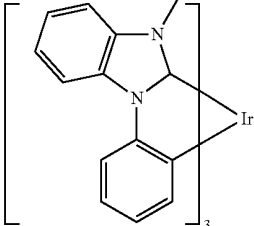
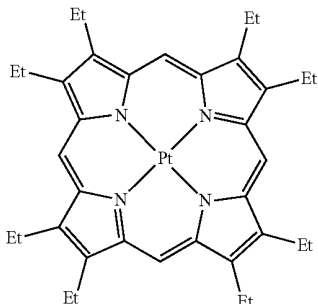
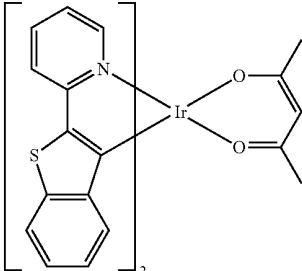
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon/ Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex		U.S. Pat. No. 7154114
Phosphorescent dopants Red dopants		
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 2-continued

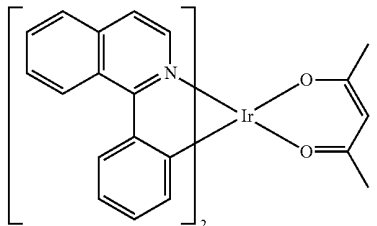
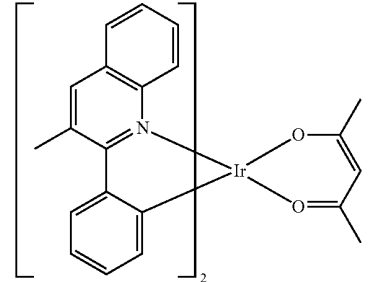
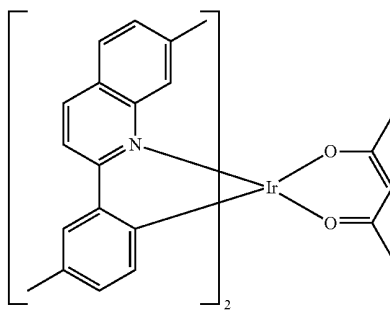
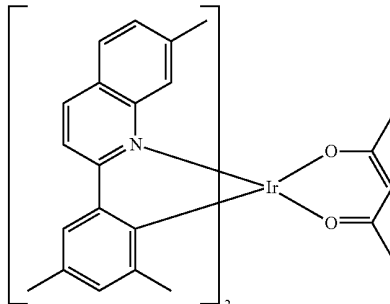
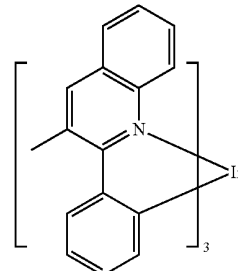
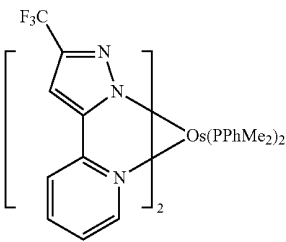
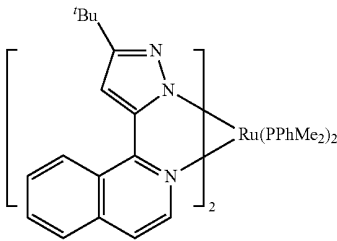
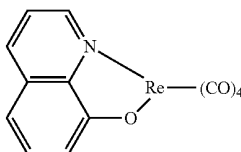
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 2006835469
		U.S. Pat. No. 2006835469
		U.S. Pat. No. 20060202194
		U.S. Pat. No. 20060202194
		U.S. Pat. No. 20070087321

TABLE 2-continued

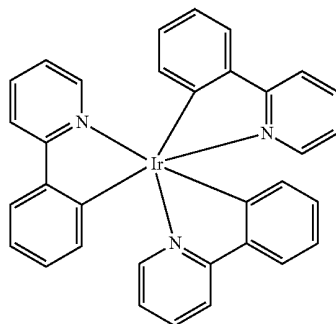
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Platinum(II) organometallic complexes		U.S. Pat. No. 20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
		WO2003040257

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		U.S. Pat. No. 20050244673

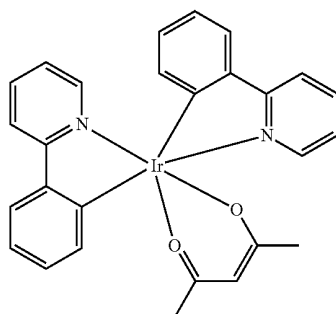
## Green dopants

Iridium(III)  
organometallic  
complexes



Inorg. Chem.  
40, 1704  
(2001)

and its derivatives



U.S. Pat. No.  
20020034656

TABLE 2-continued

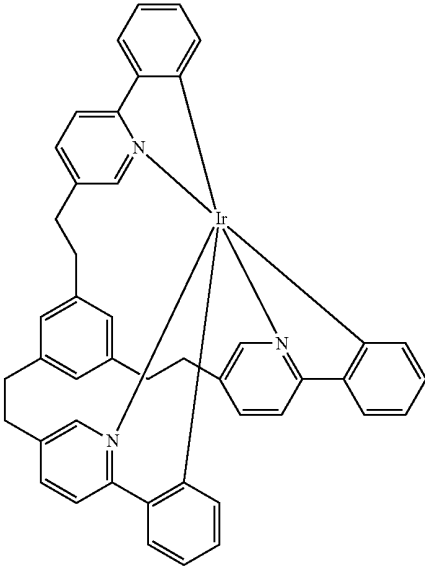
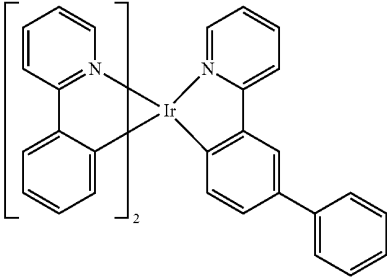
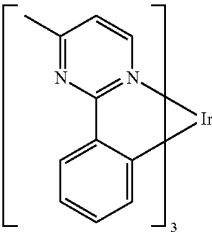
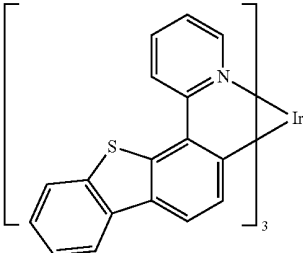
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		U.S. Pat. No. 7332232
		U.S. Pat. No. 20090108737
		U.S. Pat. No. 20090039776
		U.S. Pat. No. 6921915

TABLE 2-continued

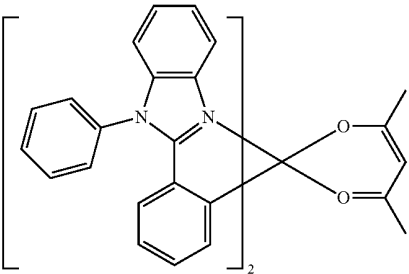
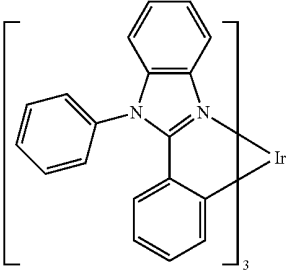
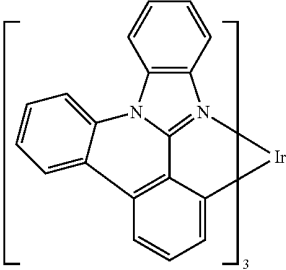
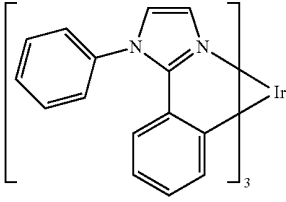
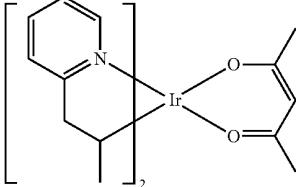
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 6687266
		Chem. Mater. 16, 2480 (2004)
		U.S. Pat. No. 20070190359
		U.S. Pat. No. 20060008670 JP2007123392
		Adv. Mater. 16, 2003 (2004)

TABLE 2-continued

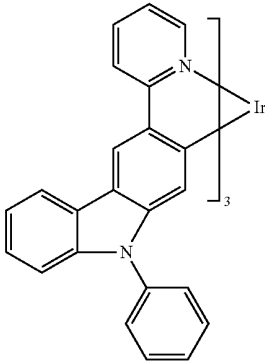
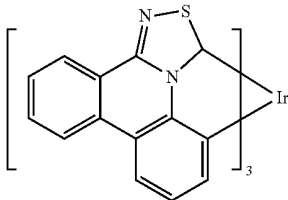
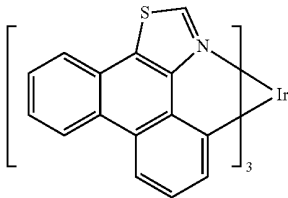
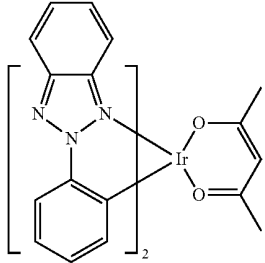
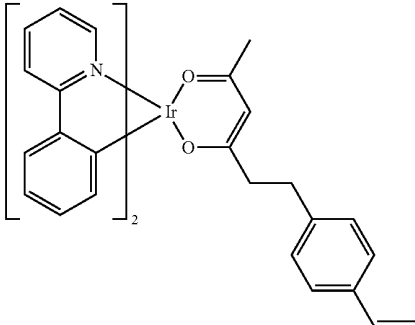
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		U.S. Pat. No. 20090165846
		U.S. Pat. No. 20080015355
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7250226, U.S. Pat. No. 7396598



TABLE 2-continued

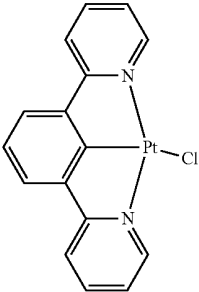
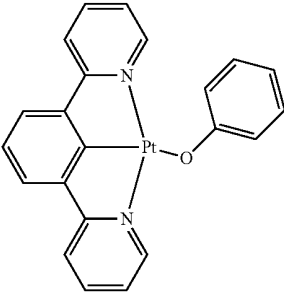
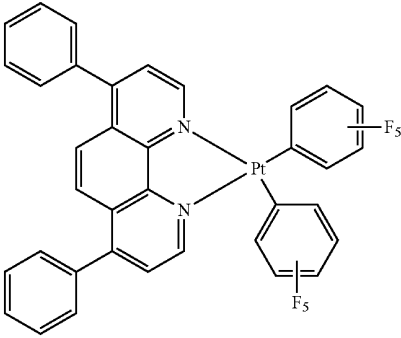
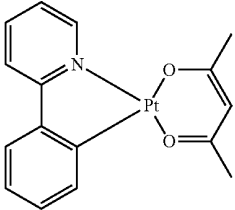
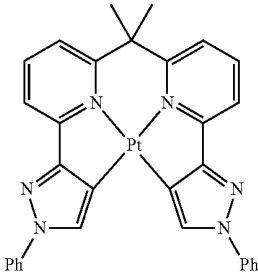
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Pt(II) organometallic complexes, including polydentate ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		U.S. Pat. No. 20060263635

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)
Deuterated organometallic complexes		U.S. Pat. No. 20030138657

TABLE 2-continued

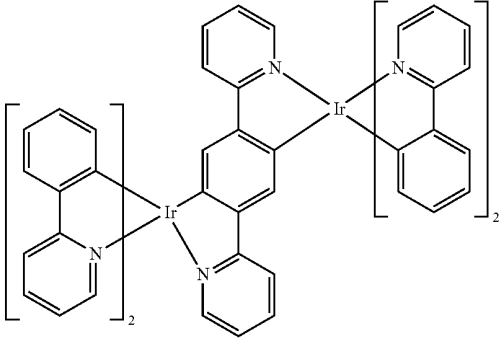
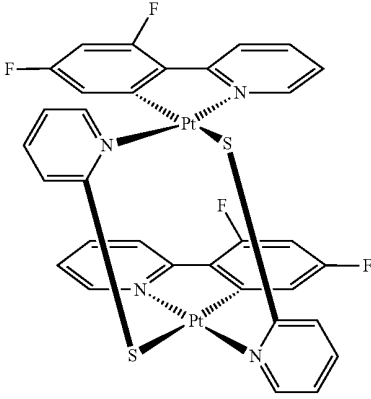
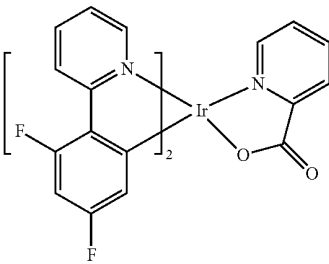
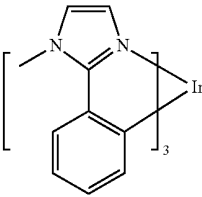
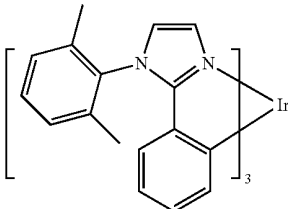
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organometallic complexes with two or more metal centers		U.S. Pat. No. 20030152802
		U.S. Pat. No. 7090928
Blue dopants		
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		U.S. Pat. No. 20060251923

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7393599, WO2006056418, U.S. Pat. No. 20050260441, WO2005019373
		U.S. Pat. No. 7534505
		U.S. Pat. No. 7445855
		U.S. Pat. No. 20070190359, U.S. Pat. No. 20080297033
		U.S. Pat. No. 7338722
		U.S. Pat. No. 20020134984

TABLE 2-continued

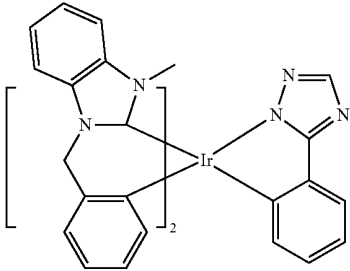
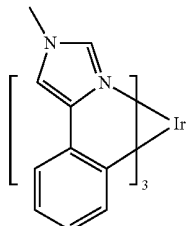
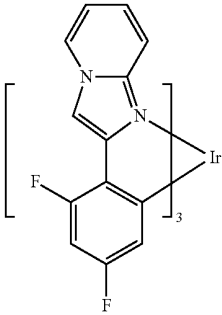
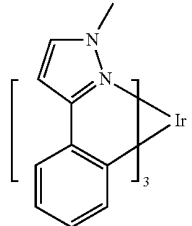
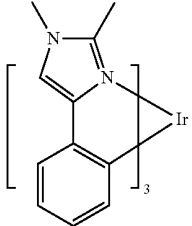
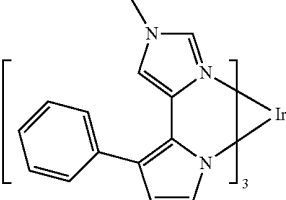
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006082742
Osmium(II) complexes		U.S. Pat. No. 7279704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Exciton/hole blocking layer materials		
Bathocuprine compounds (e.g., BCP, BPhen)	<p>The structure shows a central benzene ring fused to two pyridine rings. Each pyridine ring has a methyl group at the 2-position and a phenyl group at the 4-position.</p>	Appl. Phys. Lett. 75, 4 (1999)
	<p>The structure shows two pyridine rings connected at their 2-positions by a central benzene ring. Each pyridine ring has a phenyl group at the 4-position.</p>	Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)	<p>The structure shows an aluminum atom coordinated to three 8-quinolinolato ligands. One ligand is shown in detail with its quinoline ring system and an oxygen atom at the 8-position. The aluminum atom is also bonded to an oxygen atom, which is part of a biphenyl group.</p>	Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole	<p>The structure shows a central benzene ring connected to three 1,2,4-triazole rings. Each triazole ring is substituted with a phenyl group.</p>	Appl. Phys. Lett. 81, 162 (2002)

TABLE 2-continued

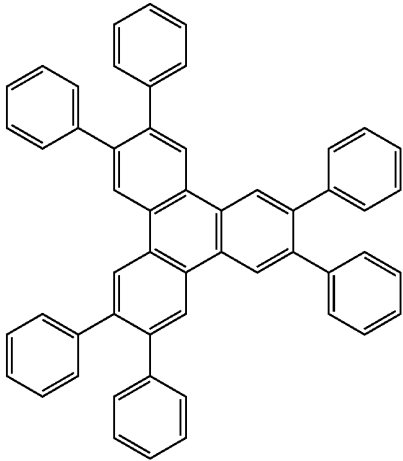
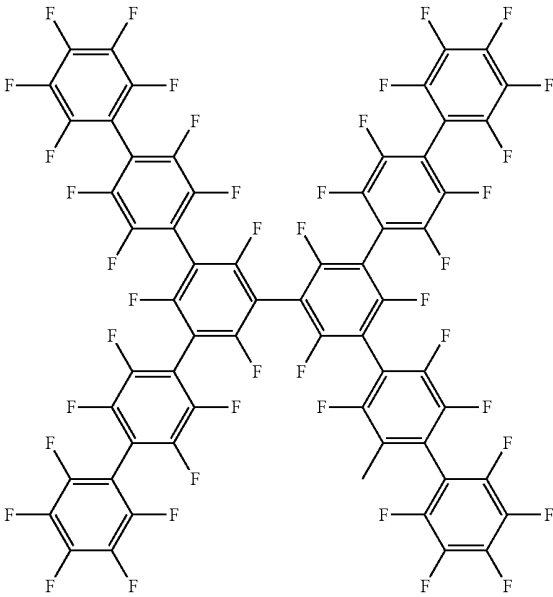
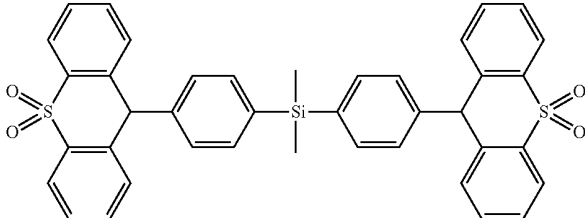
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triphenylene compounds		U.S. Pat. No. 20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085



TABLE 2-continued

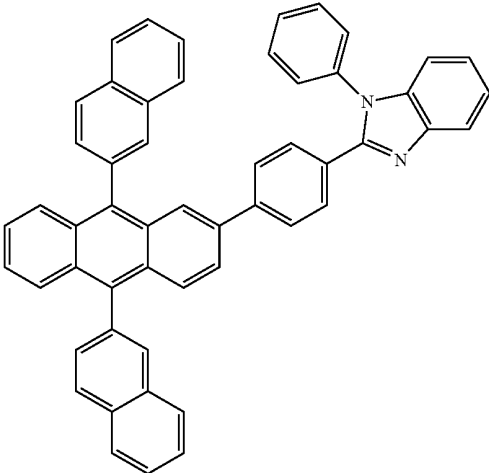
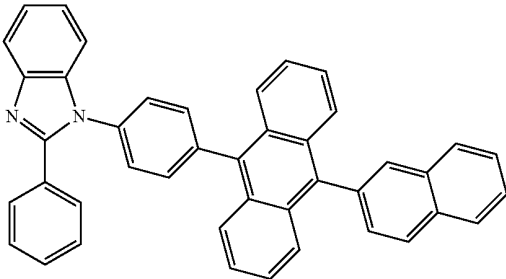
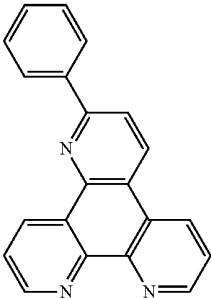
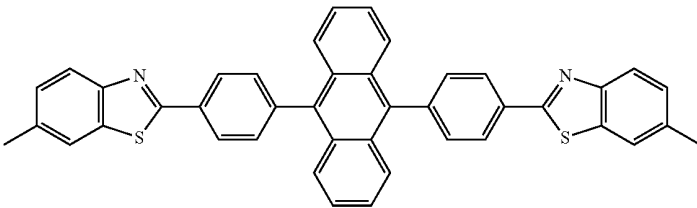
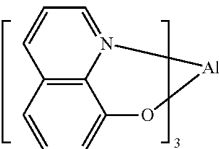
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Electron transporting materials		
Anthracene-benzimidazole compounds		WO2003060956
		U.S. Pat. No. 20090179554
Aza triphenylene derivatives		U.S. Pat. No. 20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq <sub>3</sub> , Zr <sub>q</sub> <sub>4</sub> )		Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7230107

TABLE 2-continued

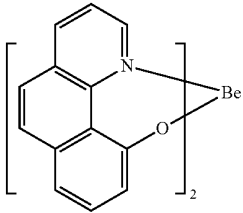
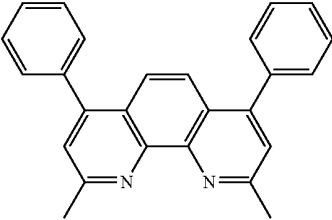
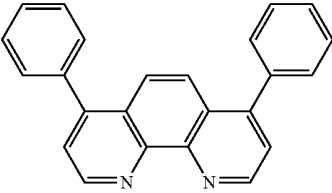
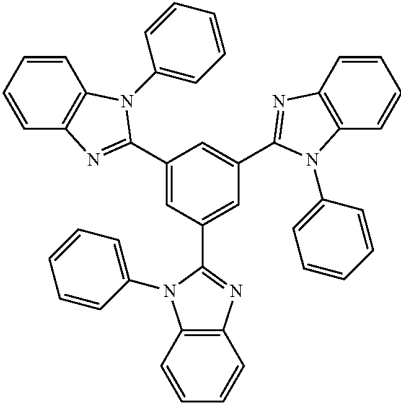
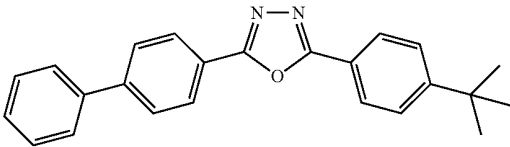
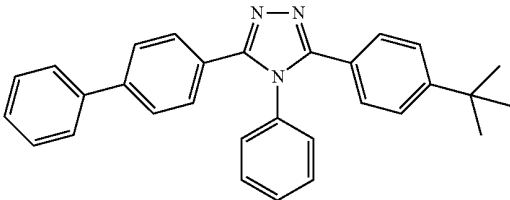
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal hydroxy-benzoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
		Appl. Phys. Lett. 79, 449 (2001)
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)

TABLE 2-continued

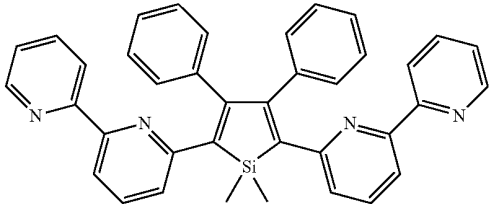
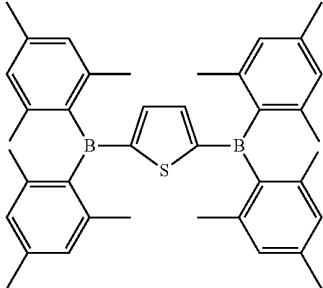
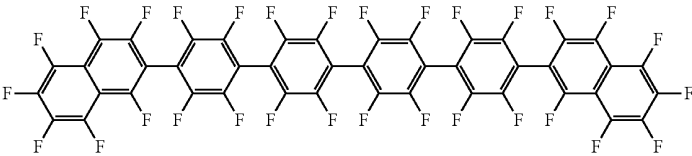
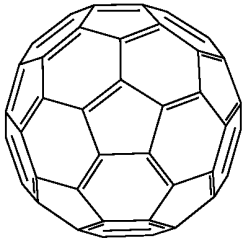
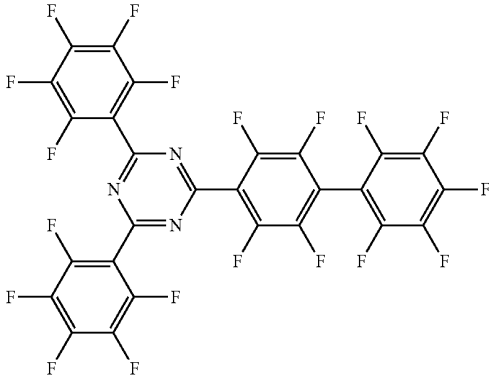
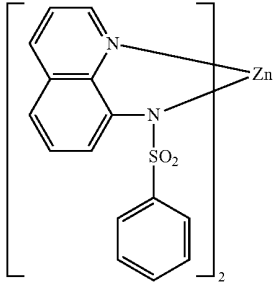
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silole compounds		Org. Electron. 4, 113  (200)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		U.S. Pat. No. 20090101870
Triazine complexes		U.S. Pat. No. 20040036077

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Zn (N <sup>-</sup> N <sup>-</sup> ) complexes		U.S. Pat. No. 6528187

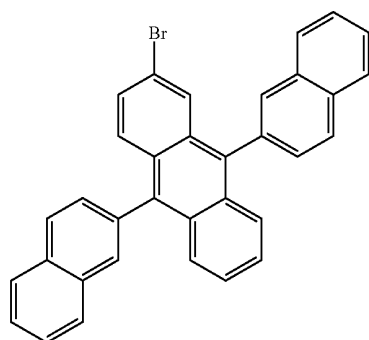
## EXPERIMENTAL

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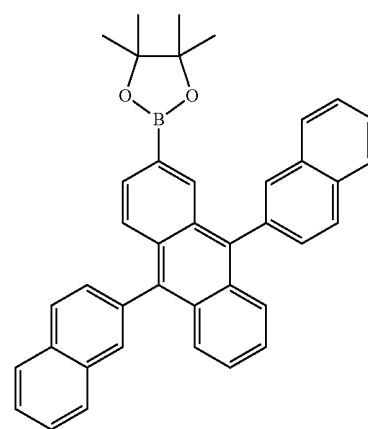
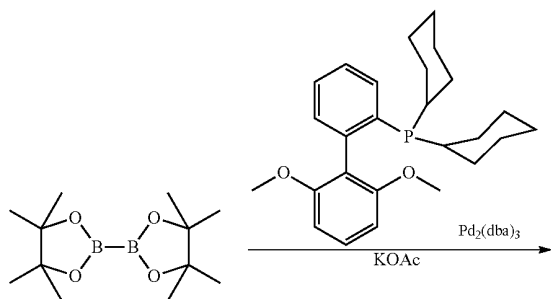
## Compound Examples

## Example 1

## Synthesis of Compound 1

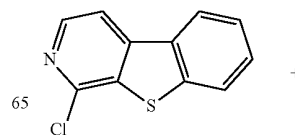


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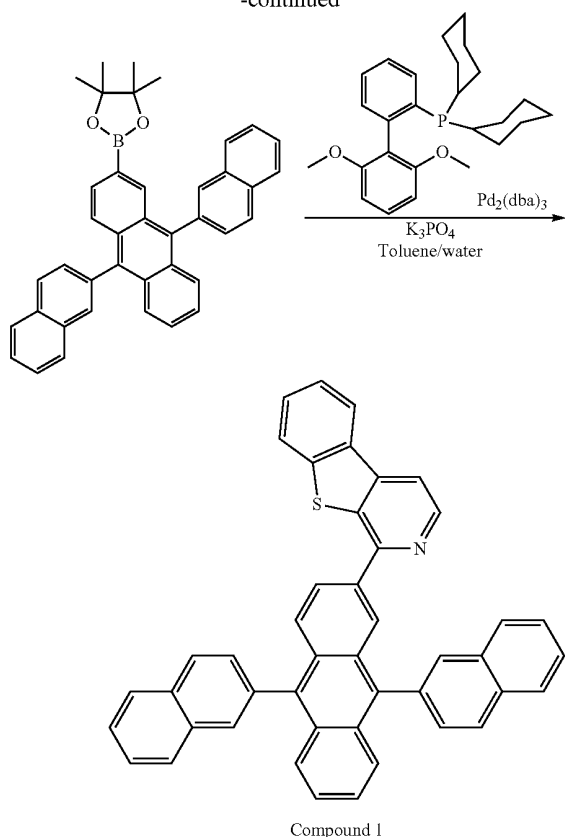
## Synthesis of 2-(9,10-di(naphthalen-2-yl)anthracen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

2-bromo-9,10-di(naphthalen-2-yl)anthracene (4.75 g, 9.32 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (3.08 g, 12.12 mmol), potassium acetate (1.830 g, 18.65 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.153 g, 0.373 mmol) were mixed in 400 mL of dioxane. The mixture was bubbled with nitrogen for 20 minutes. Pd<sub>2</sub>(dba)<sub>3</sub> (0.085 g, 0.093 mmol) was added. The reaction was heated up to 90° C. overnight. The reaction was stopped and filtered through Celite. Solvent was evaporated, coated on Celite and a column was run with 10% ethyl acetate and hexanes. The solid was then recrystallized from 100 mL of ethanol. Yellowish solid 2-(9,10-di(naphthalen-2-yl)anthracen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.8 g, 6.83 mmol, 73.2% yield) was collected by filtration.



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-continued



## Synthesis of Compound 1

A mixture of 1-chlorobenzo[4,5]thieno[2,3-c]pyridine (2.4 g, 10.93 mmol), 2-(9,10-di(naphthalen-2-yl)anthracen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.8 g, 6.83 mmol), and potassium phosphate (3.62 g, 17.07 mmol) in 200 mL of toluene and 20 mL of H<sub>2</sub>O was bubbled with N<sub>2</sub> for 20 minutes. Pd<sub>2</sub>(dba)<sub>3</sub> (0.125 g, 0.137 mmol) and dicyclohexyl (2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.224 g, 0.546 mmol) were then added, and the mixture was heated to reflux under N<sub>2</sub> for 6 h. The mixture was cooled and the solid was collected by filtration. The solid was washed with water, methanol and acetone and then dried. 3 g of solid was obtained. The solid was refluxed with 300 mL of toluene overnight under nitrogen. After it cooled to room temperature, the solid was collected by filtration. The process was repeated with another 300 mL of toluene. The solid was collected and dried under vacuum. 1-(9,10-di(naphthalen-2-yl)anthracen-2-yl)benzo[4,5]thieno[2,3-c]pyridine (3 g, 4.89 mmol, 71.6% yield) was obtained.

## Device Examples

All device examples were fabricated by high vacuum (<10<sup>-7</sup> Torr) thermal evaporation. The anode electrode is 800 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1000 Å of Al. All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H<sub>2</sub>O and O<sub>2</sub>) immediately after fabrication, and a moisture getter was incorporated inside the package.

The organic stack of the Device Examples consisted of sequentially, from the ITO surface, 100 Å of Compound A as the hole injection layer (HIL), 300 Å of 4,4'-bis[N-(1-naph-

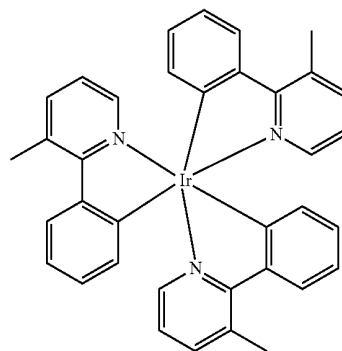
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thyl)-N-phenylamino]biphenyl (α-NPD) as the hole transporting layer (HTL), 300 Å of Host 1 doped with Compound A as the emissive layer (EML), 50 Å of Host 1 as the blocking layer (BL), and 450 Å of Compound 1 or Compound 1 doped with LiQ as the electron transport layer (ETL).

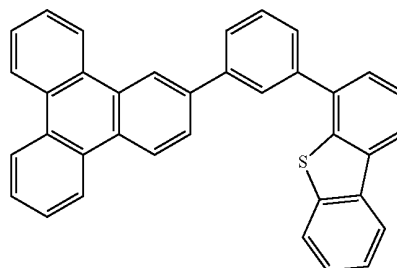
The Comparative Device Example was fabricated similarly to the Device Examples, except Alq was used as the ETL.

As used herein, the following compounds have the following structures:

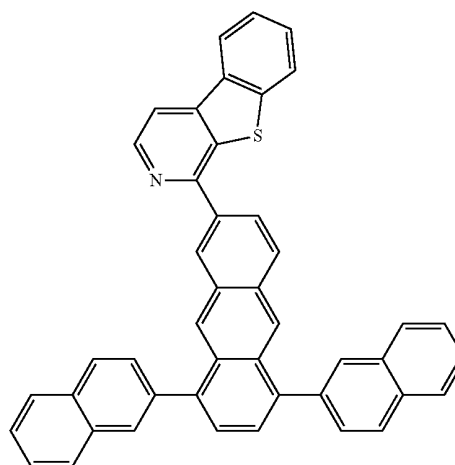
Compound A



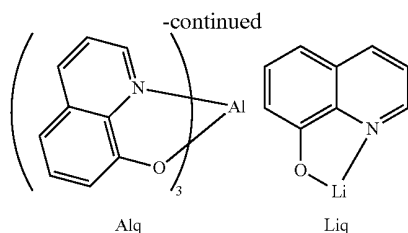
Host 1



Compound 1



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Particular compounds for the ETL of an OLED are provided. These compounds may lead to devices having particularly good properties. The device structures are provided in Table 3, and the corresponding device data is provided in Table 4. Cmpd. is an abbreviation of compound. Comp. is an abbreviation of comparative. Ex. is an abbreviation of example.

TABLE 3

VTE PHOLEDs					
Example	HIL	HTL	EML (doping %)	BL	ETL
Ex. 1	Cmpd. A	NPD	Host 1	Cmpd. A 10%	Host 1
Ex. 2	Cmpd. A	NPD	Host 1	Cmpd. A 10%	Host 1
Comp. Ex. 1	Cmpd. A	NPD	Host 1	Cmpd. A 10%	Alq

TABLE 4

VTE device data									
Example	1931 CIE		At 1000 nits				At 40 mA/cm <sup>2</sup>		
	x	y	$\lambda_{max}$	V (V)	LE (Cd/A)	EQE (%)	PE (lm/W)	L <sub>0</sub> (nits)	LT <sub>80%</sub> (h)
Ex. 1	0.35	0.60	528	7.8	41.5	11.4	16.6	13,566	217
Ex. 2	0.34	0.61	528	6.2	45.2	12.4	22.8	15,853	224
Comp. Ex. 1	0.35	0.60	528	8.1	45.6	12.5	17.7	15,780	221

Device Examples 1 and 2 showed green PHOLEDs with Compound 1 or Compound 1 doped with LiQ as the ETL. Comparative Example 1 used Alq as the ETL. As can be seen from the tables, Device Examples 1 and 2 with Compound 1 or Compound 1 doped with LiQ as the ETL, respectively, had similar efficiency and device lifetime as compared with Comparative Device Example 1 with Alq as the ETL. However, the device operating voltage of Device Example 1 was lower than the operating voltage of Comparative Example 1, i.e., 7.8 V compared to 8.1 V. The operating voltage of Device Example 2 was even further decreased to 6.2 V. Therefore, devices comprising an inventive compound as the ETL may maintain good lifetime and efficiency and have lowered device voltage.

It is understood that the various embodiments described herein by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

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The invention claimed is:

1. A compound having the formula  $\text{Ar}(\text{LiDi})_n$ , wherein Ar contains a condensed aromatic ring system having at least three benzene rings and the condensed aromatic ring has a triplet energy lower than 440 nm; wherein Ar is unsubstituted or substituted with one or more groups selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, and aryl;

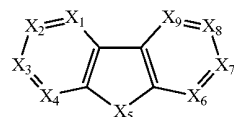
wherein L is a single bond or a bivalent linking group;

wherein n is at least 1;

wherein i is an indexing variable that identifies n structures for  $\text{L}_i$  and  $\text{D}_i$  that may be the same or different for different values of i;

wherein each  $\text{L}_i$  is independently a single bond or a bivalent linking group;

wherein each  $\text{D}_i$  independently has the structure;



wherein  $\text{X}_5$  is O, S or Se;

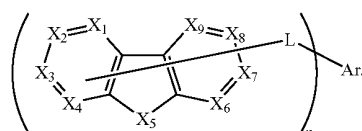
where each of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is independently selected from C(R) or N;

wherein at least one of  $\text{X}_1$ ,  $\text{X}_2$ ,  $\text{X}_3$ ,  $\text{X}_4$ ,  $\text{X}_6$ ,  $\text{X}_7$ ,  $\text{X}_8$ , and  $\text{X}_9$  is N;

wherein each R is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl; and

wherein R is optionally bound to L.

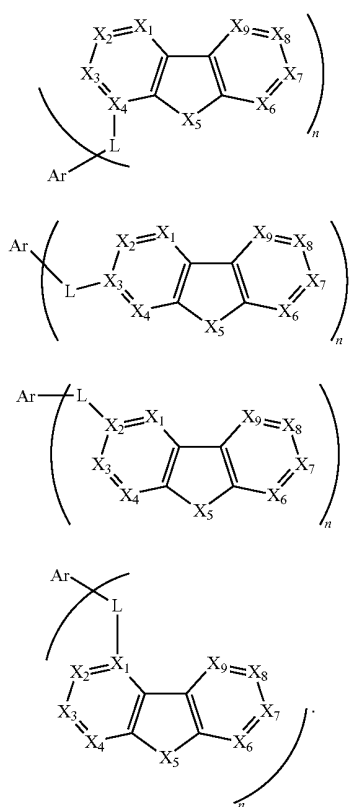
2. The compound of claim 1, wherein the compound has the formula:



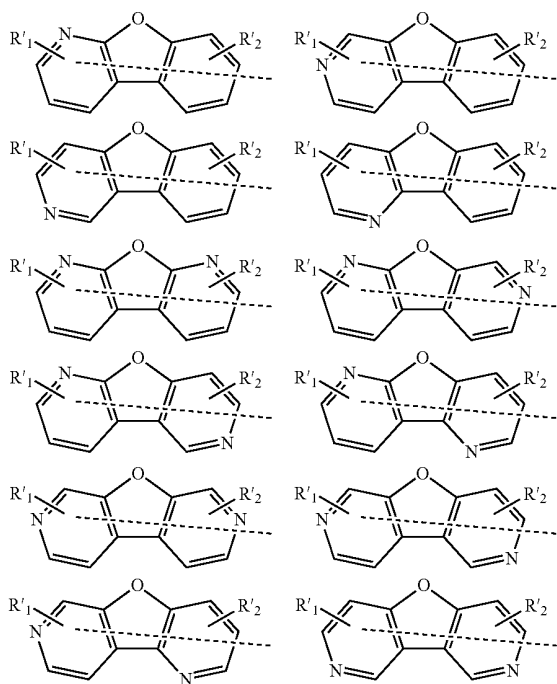
Formula I

3. The compound of claim 1, wherein the compound has a formula selected from the group consisting of:

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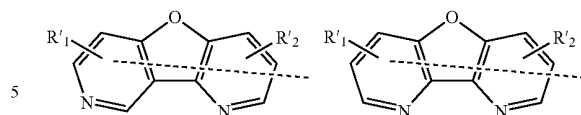
4. The compound of claim 1, wherein each  $D_i$  is independently selected from the group consisting of:



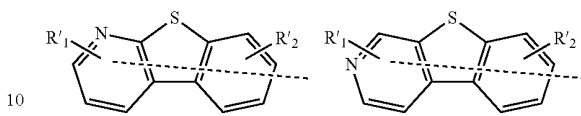
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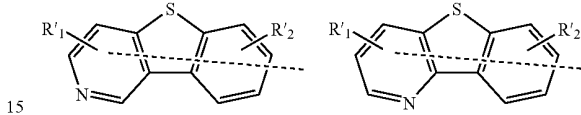
Formula II



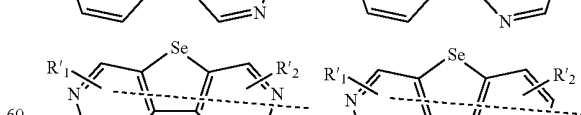
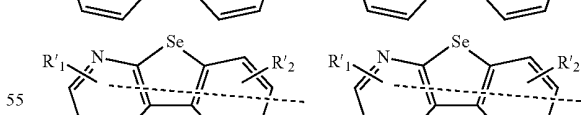
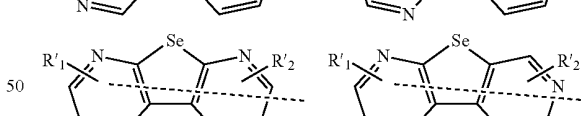
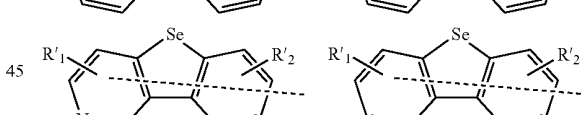
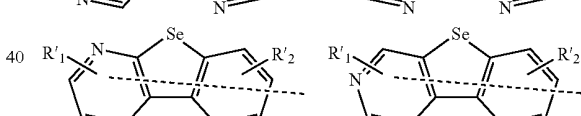
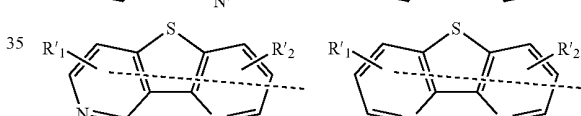
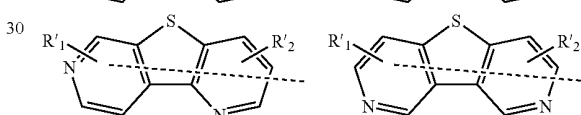
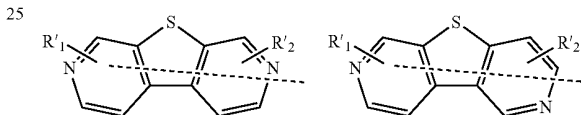
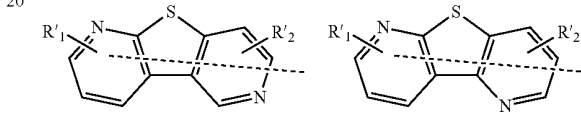
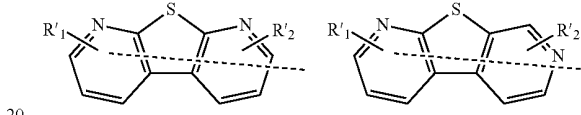
Formula III



Formula IV

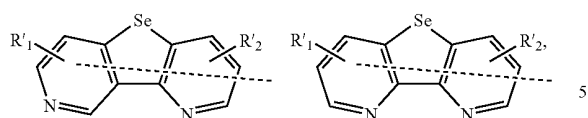


Formula V



**147**

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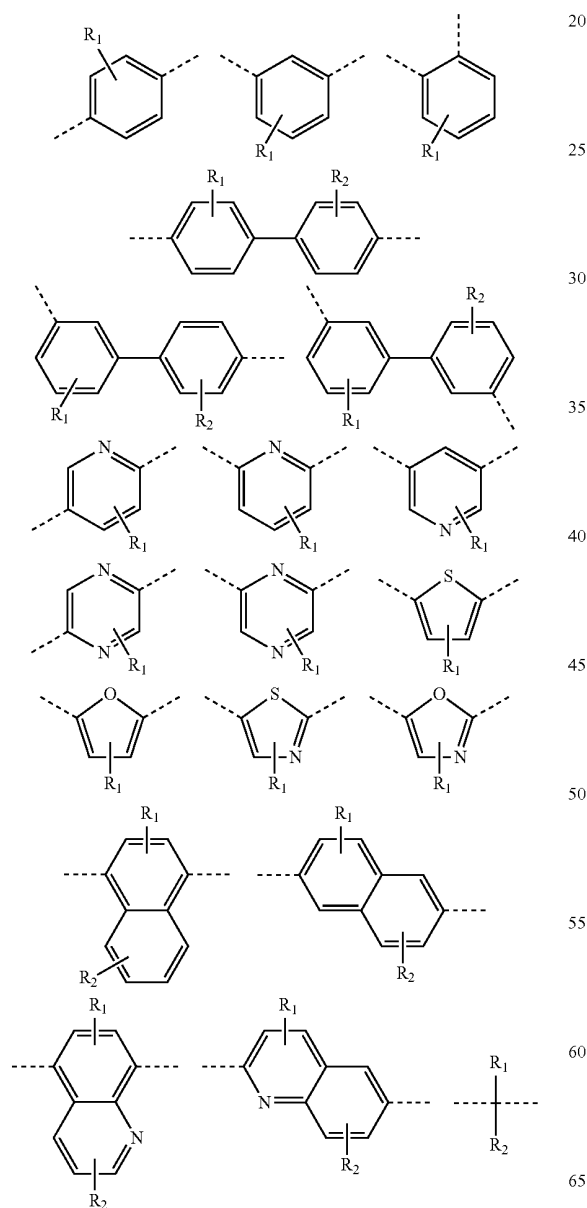


wherein  $R'_1$  and  $R'_2$  may represent mono, di, tri, or tetra substitutions; and

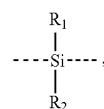
wherein  $R'_1$  and  $R'_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

5. The compound of claim 1, wherein L is a single bond.

6. The compound of claim 1, wherein each  $L_i$  is independently selected from the group consisting of:

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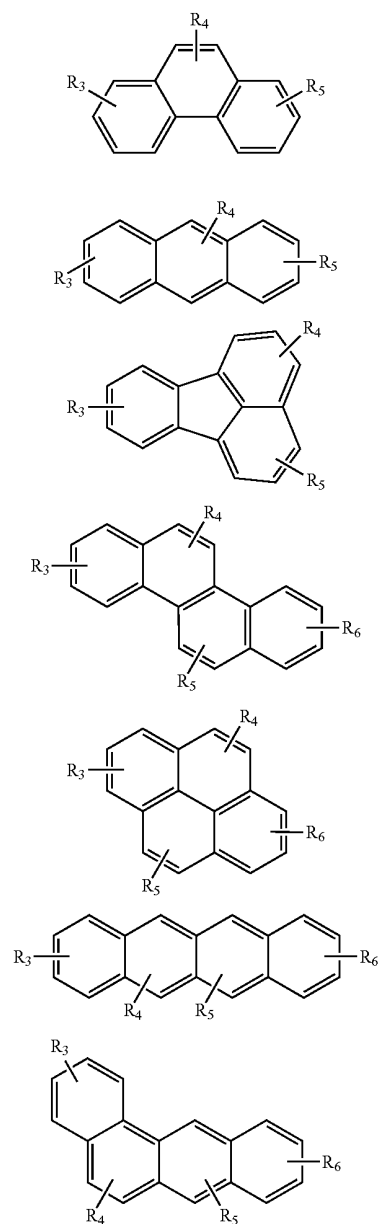
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wherein  $R_1$  and  $R_2$  may represent mono, di, tri, or tetra substitutions; and

wherein  $R_1$  and  $R_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

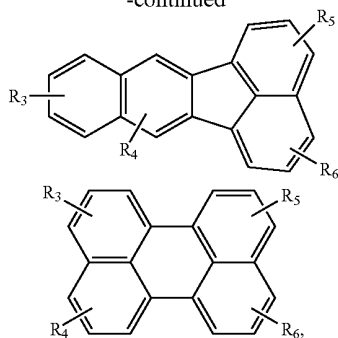
7. The compound of claim 1, wherein Ar is selected from the group consisting of:





**149**

-continued



wherein  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  may represent mono, di, tri, or tetra substitutions; and

wherein  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, and aryl.

8. The compound of claim 1, wherein  $n$  is 1.

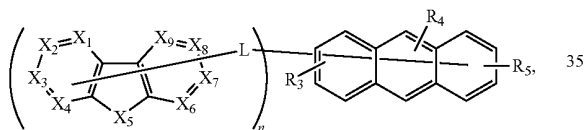
9. The compound of claim 1, wherein  $n$  is greater than 1 and each  $D_i$  has the same structure.

10. The compound of claim 1, wherein  $n$  is greater than 1 and at least two  $D_i$  have different structures.

11. The compound of claim 1, wherein  $n$  is 2.

12. The compound of claim 1, wherein the compound has the formula:

Formula VI

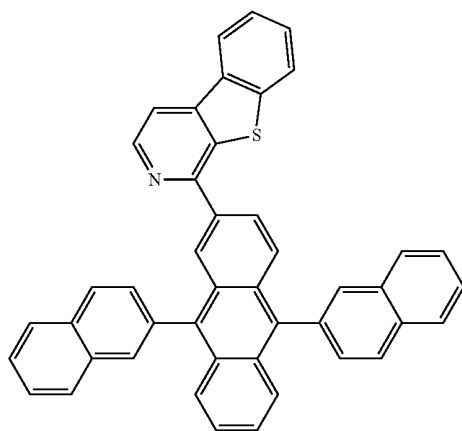


wherein  $R_3$ ,  $R_4$ , and  $R_5$  may represent mono, di, tri, or tetra substitutions; and

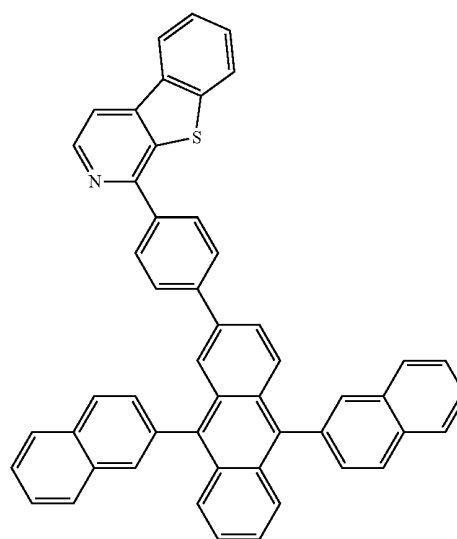
wherein  $R_3$ ,  $R_4$ , and  $R_5$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

13. The compound of claim 1, wherein the compound is selected from the group consisting of:

Compound 1

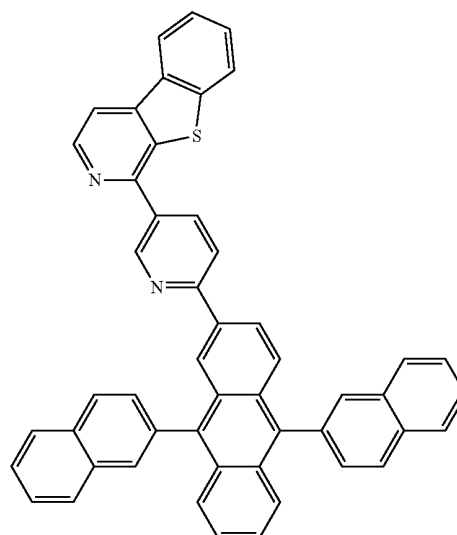
**150**

-continued

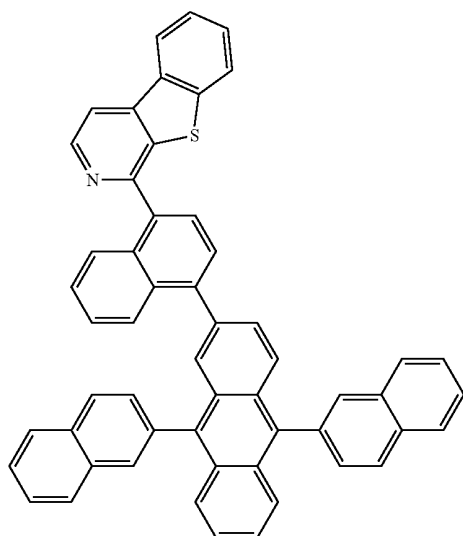


Compound 2

Compound 3



**151**  
-continued



Compound 4

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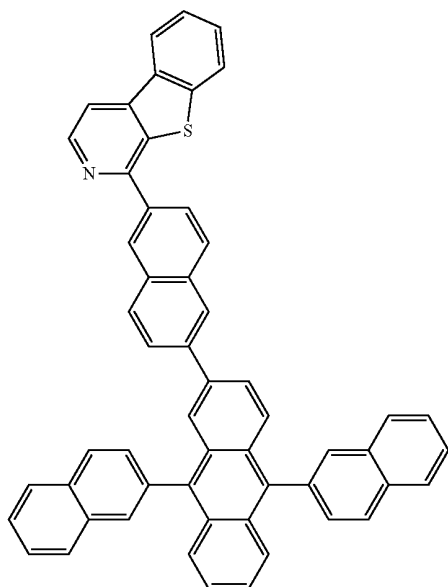
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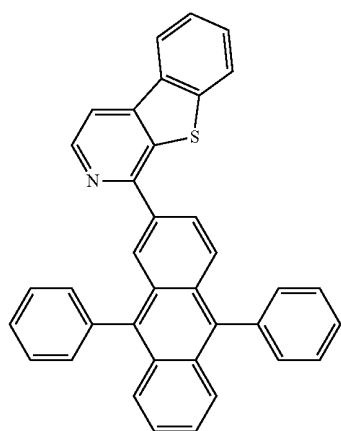
Compound 5

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Compound 6

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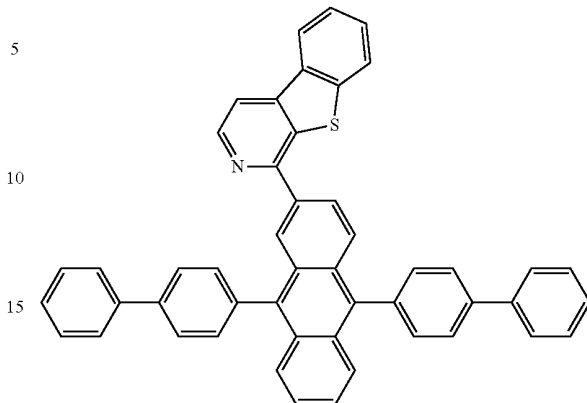
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**152**  
-continued

Compound 7



Compound 8

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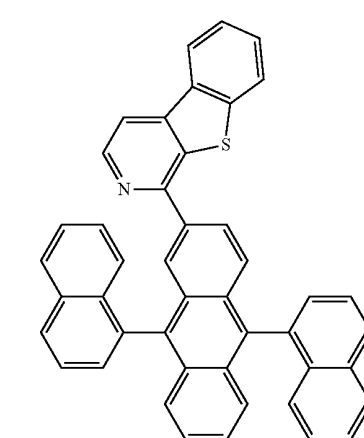
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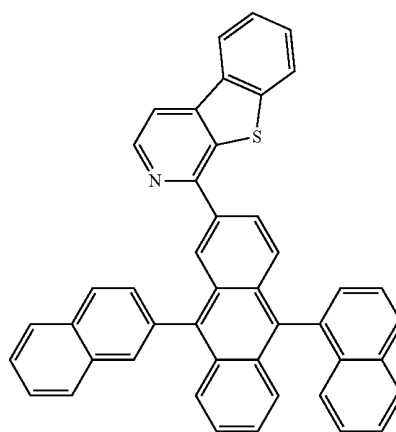
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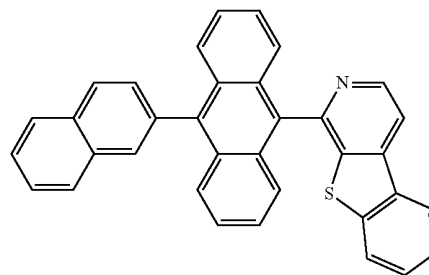
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Compound 9



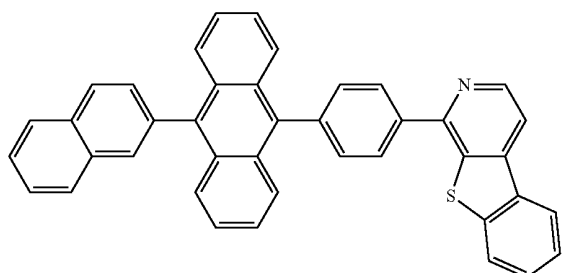
Compound 10



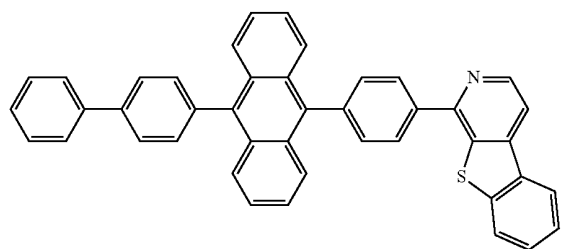
**153**

-continued

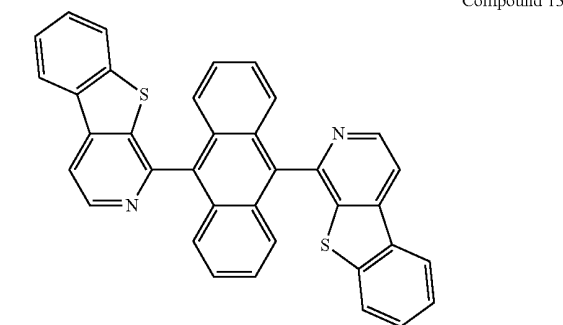
Compound 11



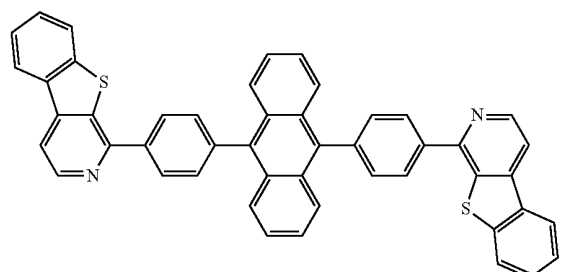
Compound 12



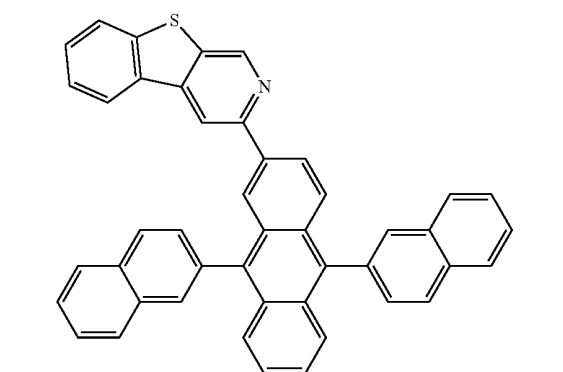
Compound 13



Compound 14

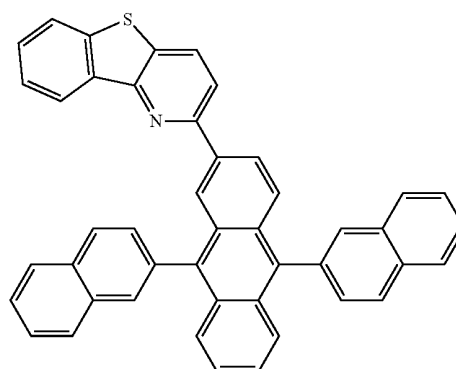


Compound 15

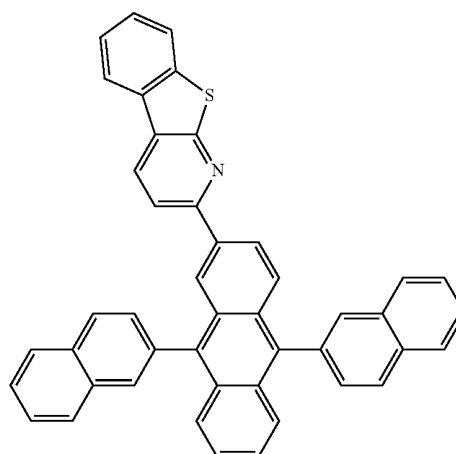
**154**

-continued

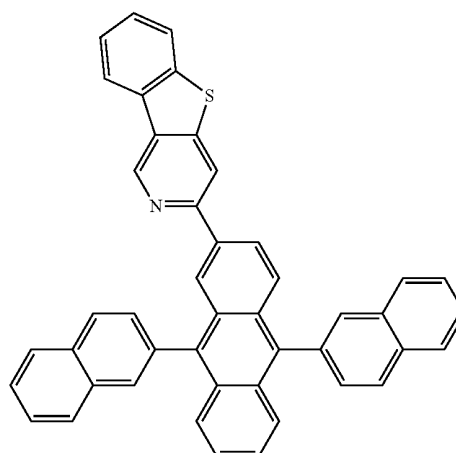
Compound 16



Compound 17

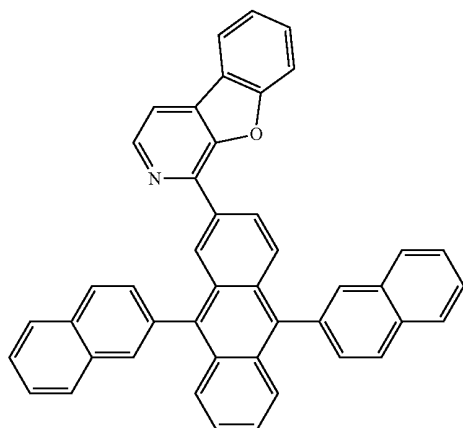


Compound 18

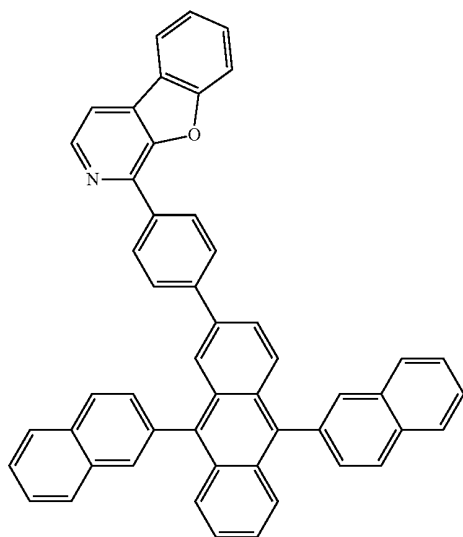


**155**  
-continued

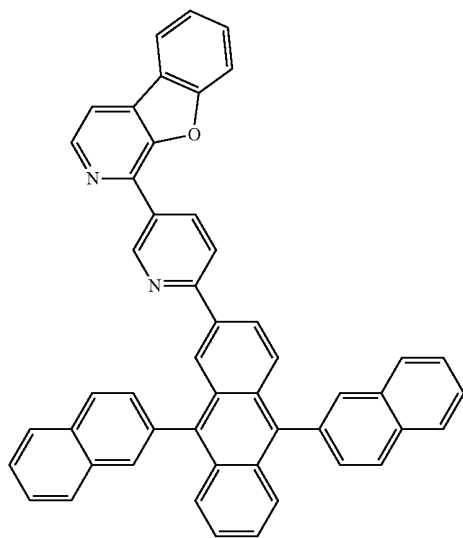
Compound 19



Compound 20

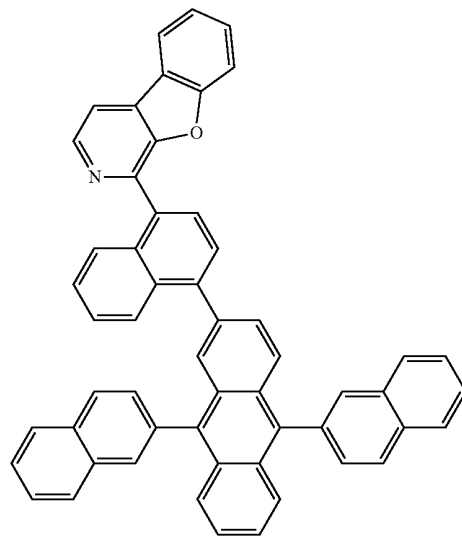


Compound 21

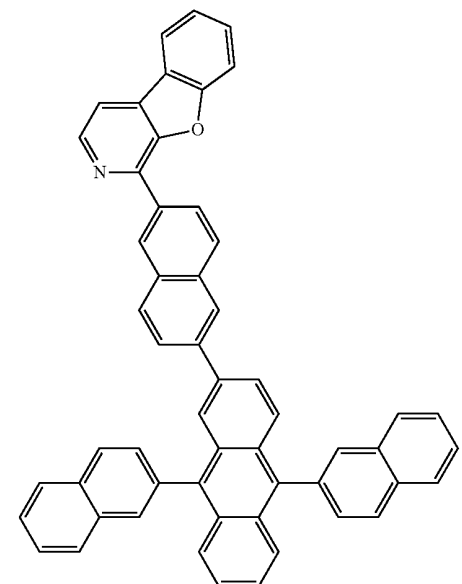


**156**  
-continued

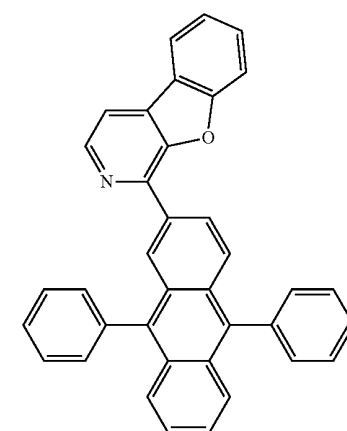
Compound 22



Compound 23

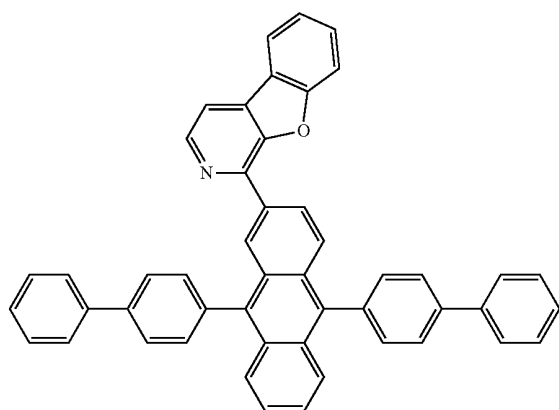


Compound 24

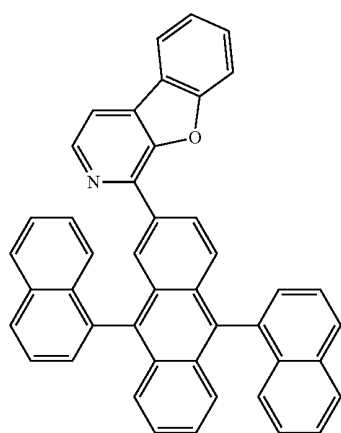


**157**

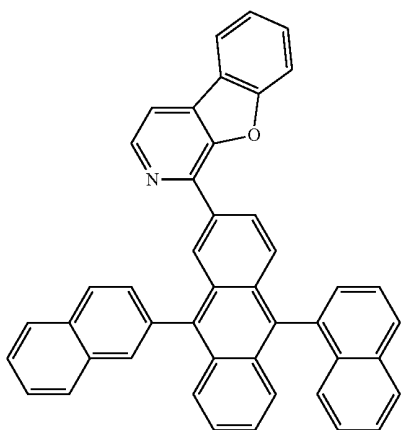
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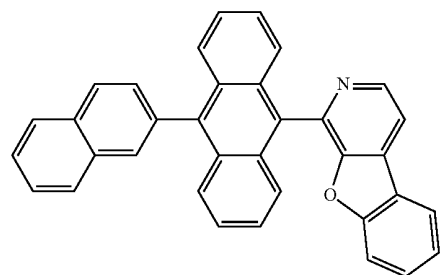
Compound 25



Compound 26



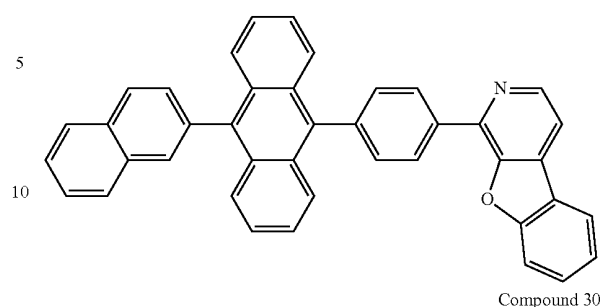
Compound 27



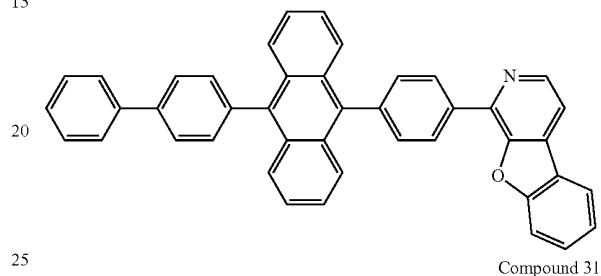
Compound 28

**158**

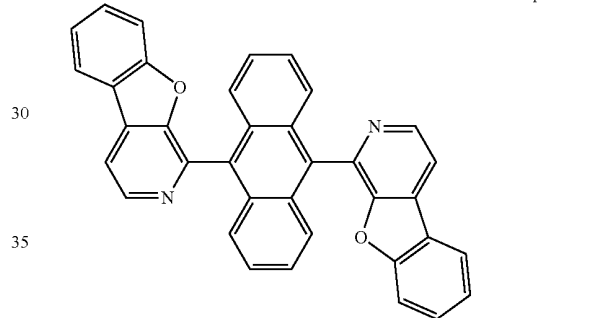
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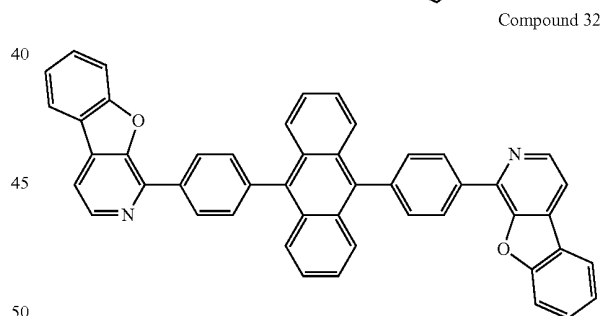
Compound 29



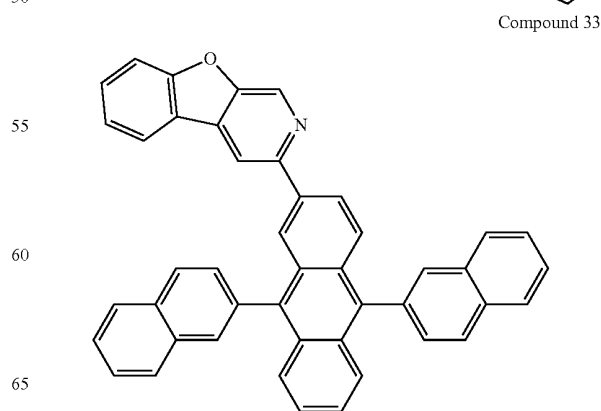
Compound 30



Compound 31



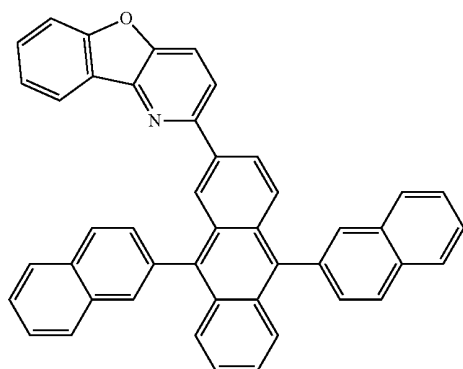
Compound 32



Compound 33

**159**  
-continued

Compound 34



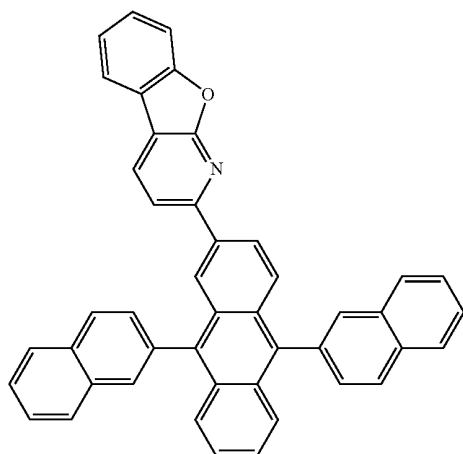
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Compound 35



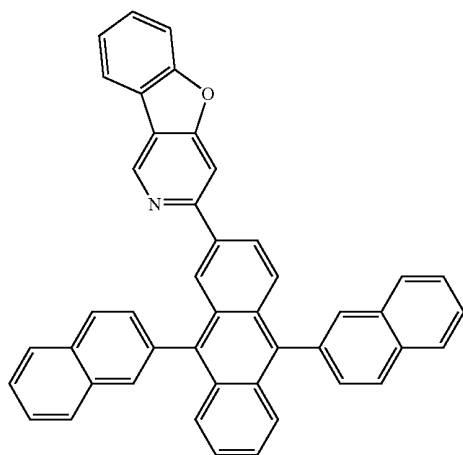
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Compound 36



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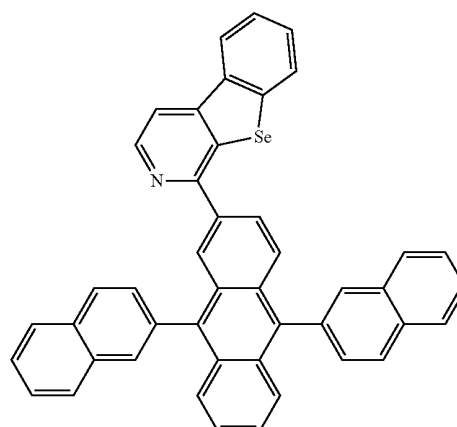
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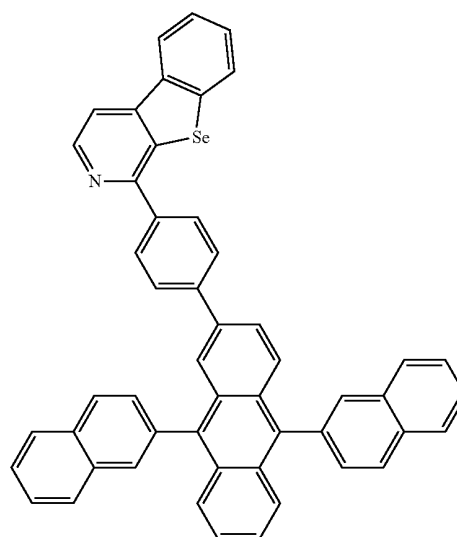
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**160**  
-continued

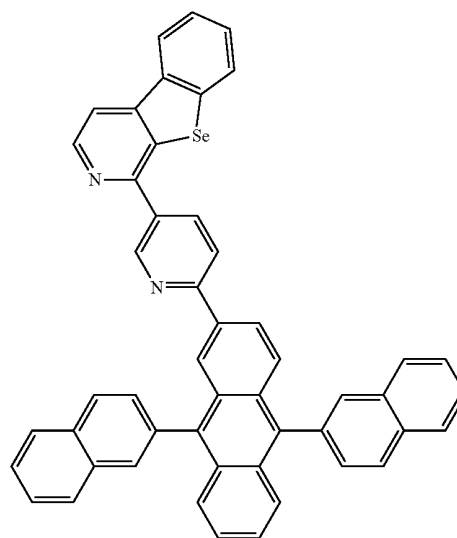
Compound 37



Compound 38

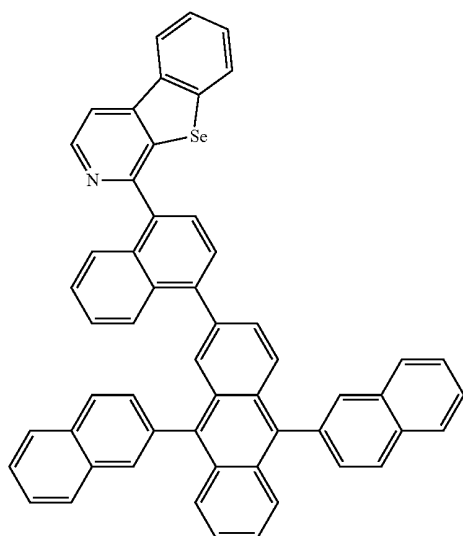


Compound 39



**161**

-continued



Compound 40

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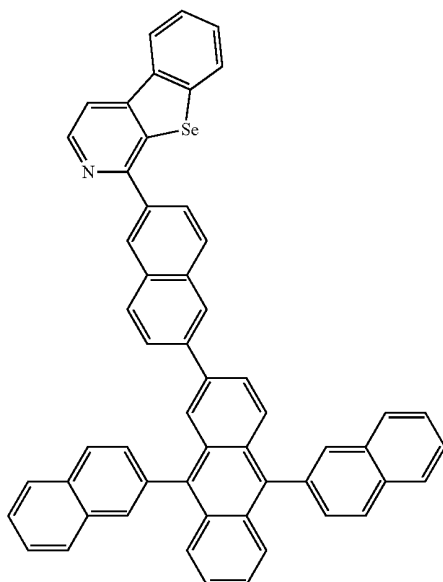
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Compound 41

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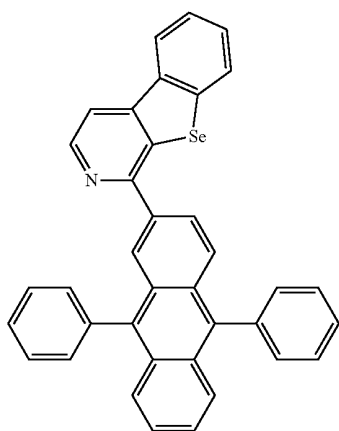
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Compound 42

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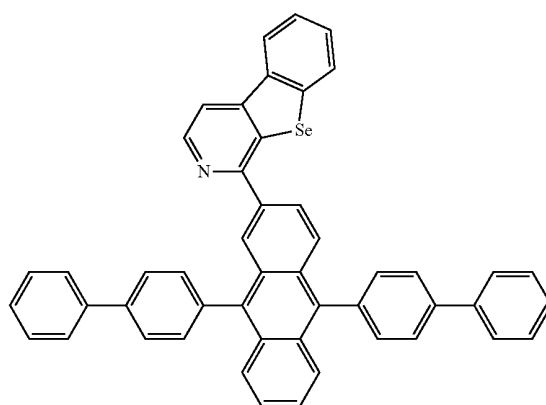
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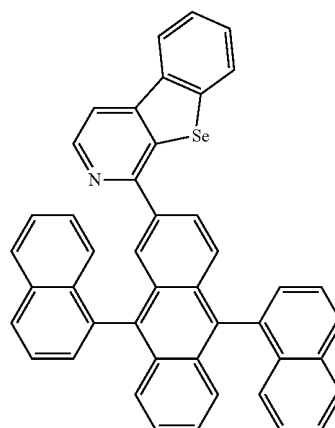
**162**

-continued

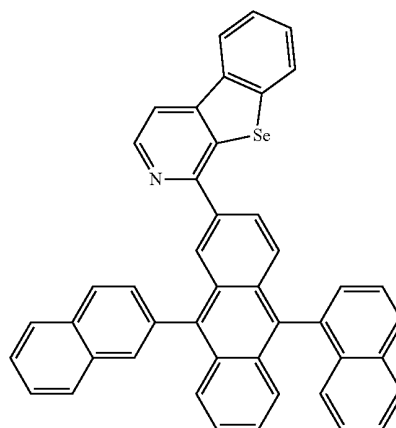


Compound 43

Compound 44



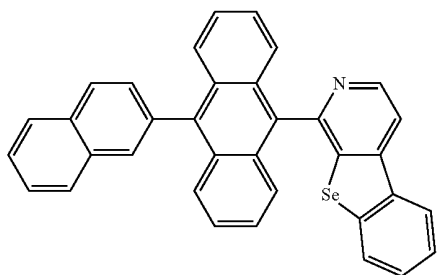
Compound 45



**163**

-continued

Compound 46

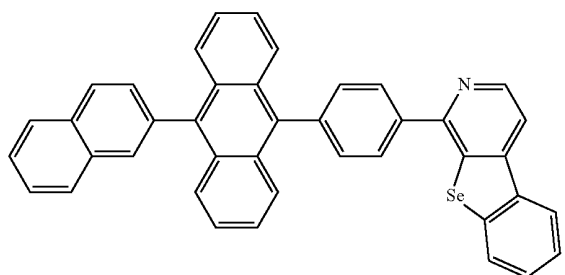


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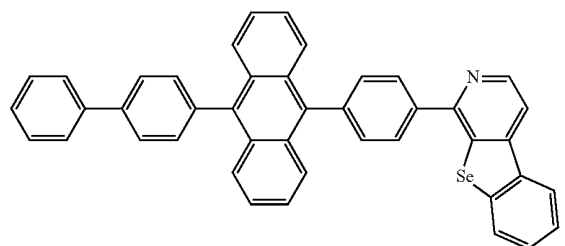
Compound 47



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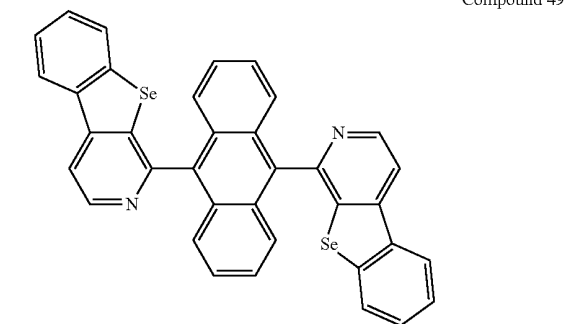
Compound 48



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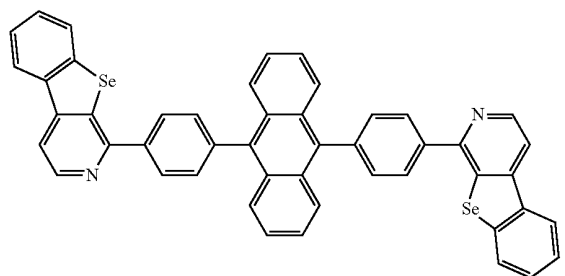
Compound 49



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Compound 50



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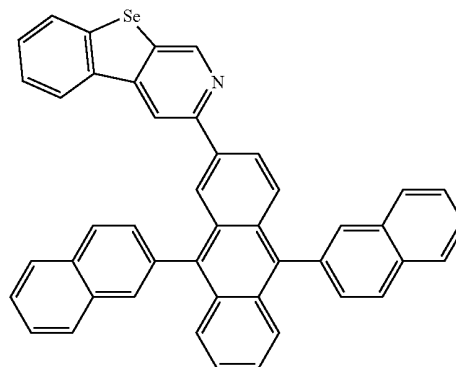
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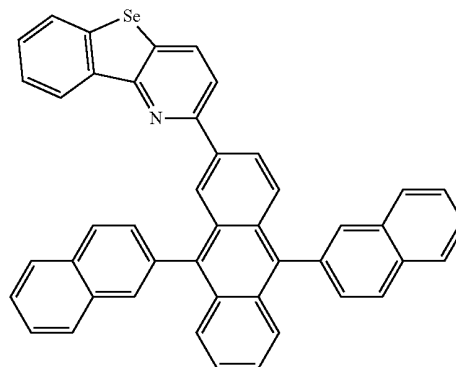
**164**

-continued

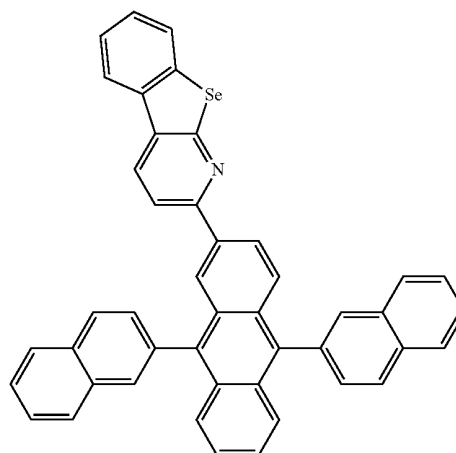
Compound 51



Compound 52

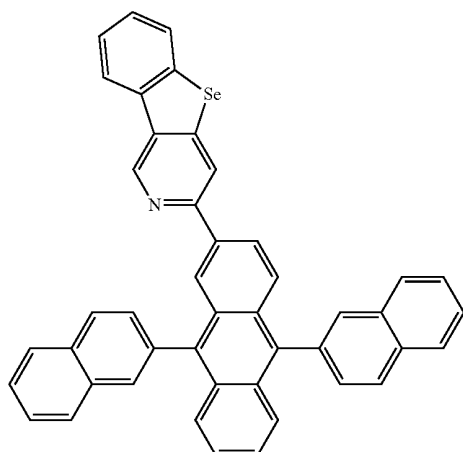


Compound 53

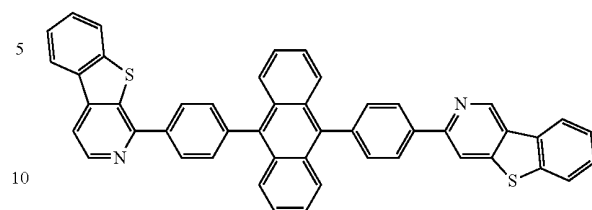




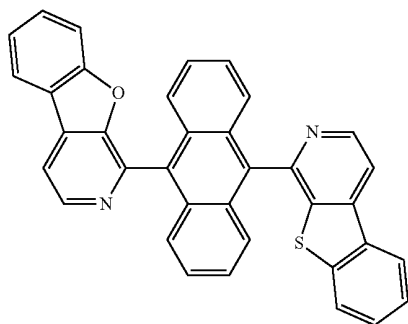
**165**  
-continued



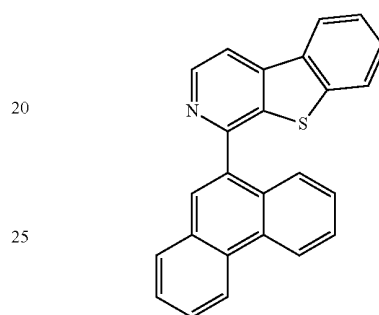
Compound 54



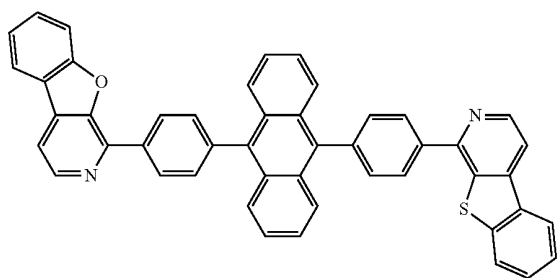
Compound 58



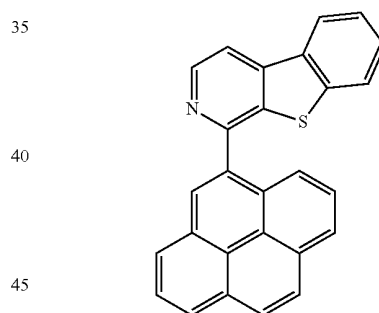
Compound 55



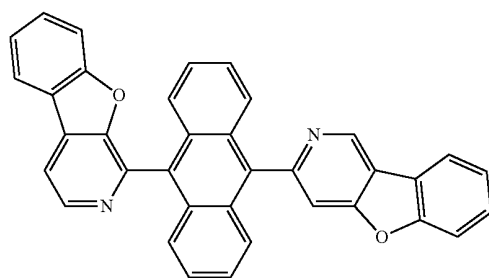
Compound 59



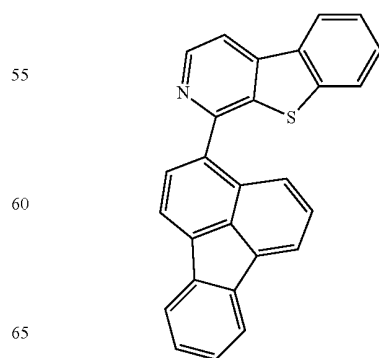
Compound 56



Compound 60



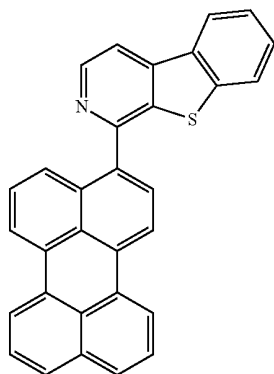
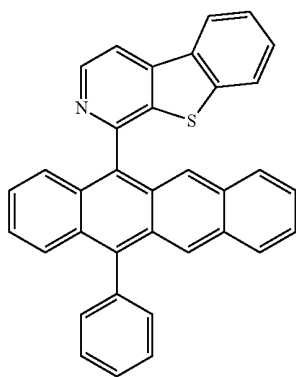
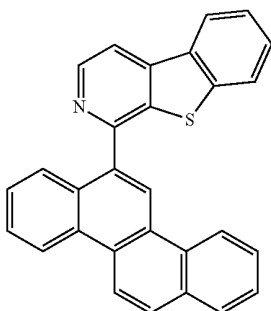
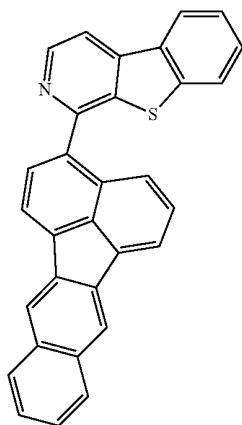
Compound 57



Compound 61

167

-continued



14. A first device comprising an organic light emitting device, comprising:  
an anode;  
a cathode; and

168

Compound 62

an organic layer, disposed between the anode and the cathode, further comprising a compound having the formula  $\text{Ar}(\text{LiDi})_n$ ,

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wherein Ar contains a condensed aromatic ring system having at least three benzene rings and the condensed aromatic ring has a triplet energy lower than 440 nm;

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wherein Ar is unsubstituted or substituted with one or more groups selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, and aryl;

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wherein L is a single bond or a divalent linking group;

wherein n is a least 1;

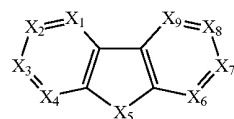
wherein i is an indexing variable that identifies n structures for  $L_i$  and  $D_i$  that may be the same or different for different values of i;

wherein each  $L_i$  is independently a single bond or a bivalent linking group;

Compound 63

wherein each  $D_i$  independently has the structure:

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wherein X, is O, S or Se;

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wherein each of  $X_1$ ,  $X_2$ ,  $X_3$ ,  $X_4$ ,  $X_6$ ,  $X_7$ ,  $X_8$ , and  $X_9$  is independently selected from C(R) or N;

Compound 64

wherein at least one of  $X_1$ ,  $X_2$ ,  $X_3$ ,  $X_4$ ,  $X_6$ ,  $X_7$ ,  $X_8$ , and  $X_9$  is N;

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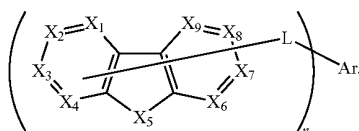
wherein each R is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl; and wherein R is optionally bound to L.

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15. The first device of claim 14, wherein the compound has the formula:

Formula I

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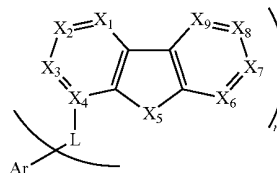
Compound 65

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16. The first device of claim 14, wherein the compound has a formula selected from the group consisting of:

Formula II

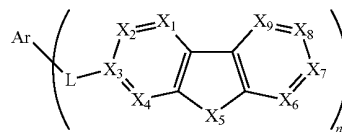
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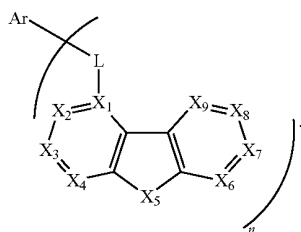
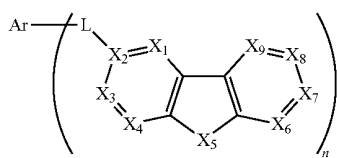
Formula III

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169

-continued

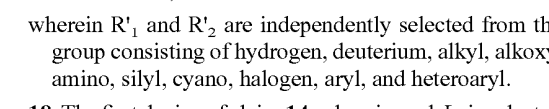
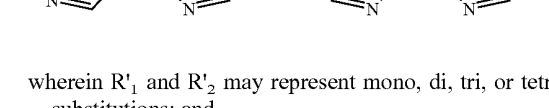
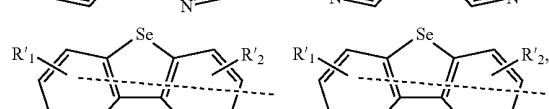
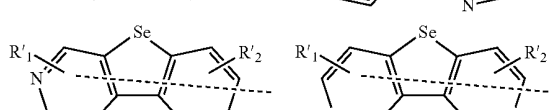
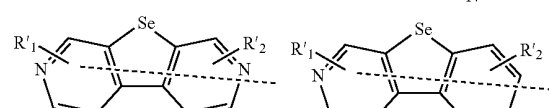
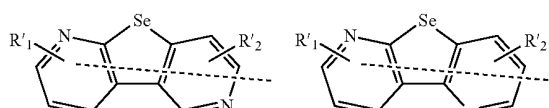
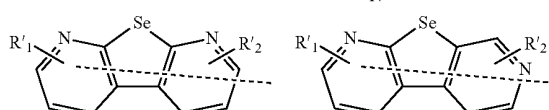
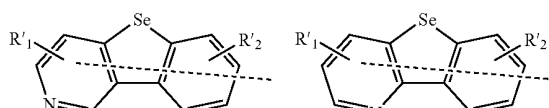
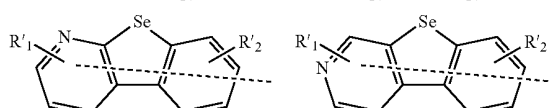
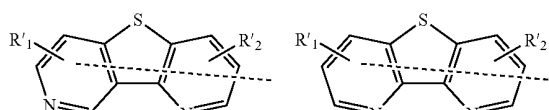
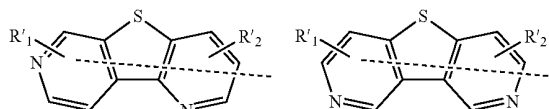
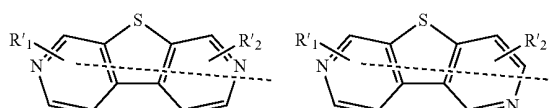
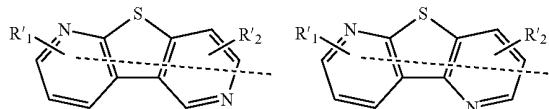
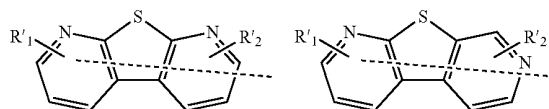


Formula IV

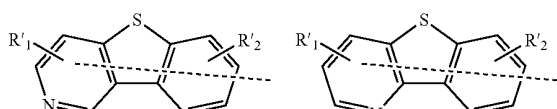
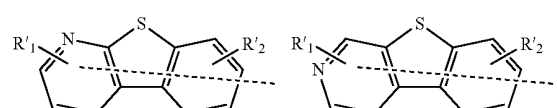
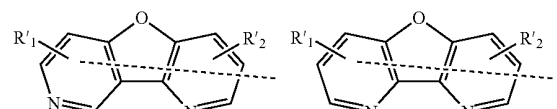
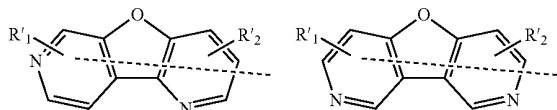
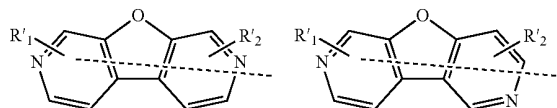
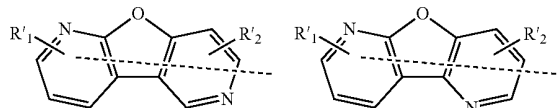
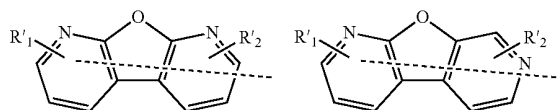
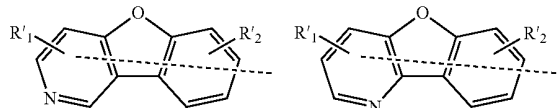
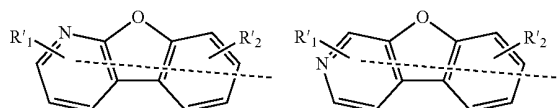
Formula V

170

-continued



17. The first device of claim 14, wherein each  $D_i$  is independently selected from the group consisting of:

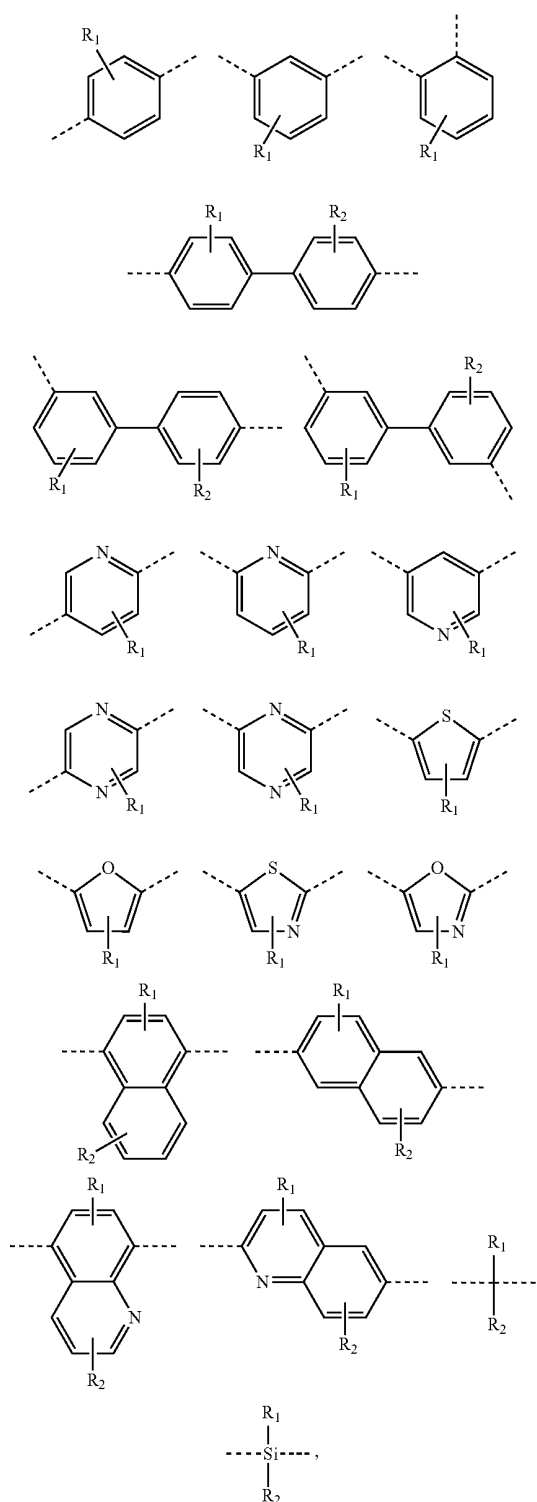


wherein  $R'_1$  and  $R'_2$  may represent mono, di, tri, or tetra substitutions; and

wherein  $R'_1$  and  $R'_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

18. The first device of claim 14, wherein each  $L_i$  is selected from the group consisting of:

171

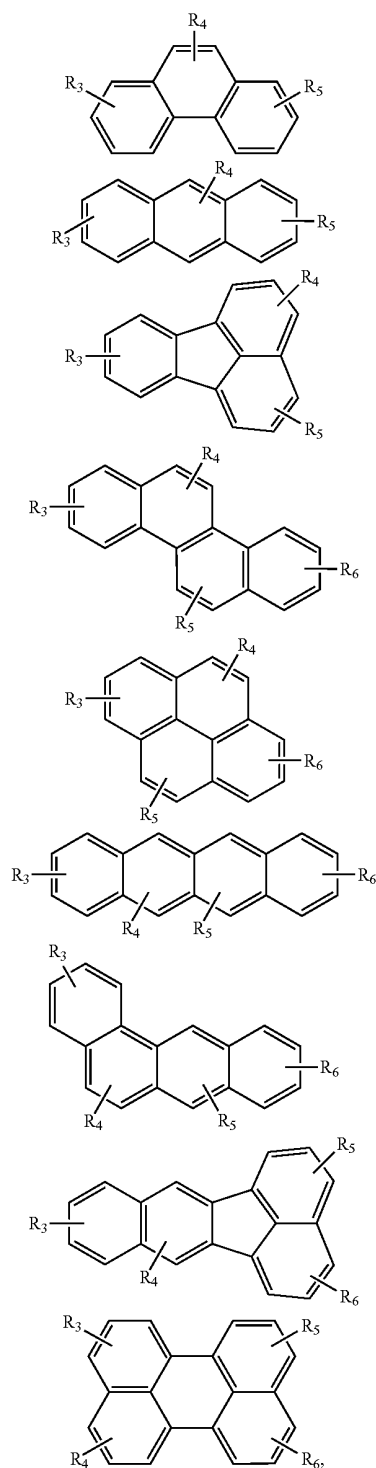


wherein  $R_1$  and  $R_2$  may represent mono, di, tri, or tetra substitutions; and

wherein  $R_1$  and  $R_2$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

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19. The first device of claim 14, wherein Ar is selected from the group consisting of:

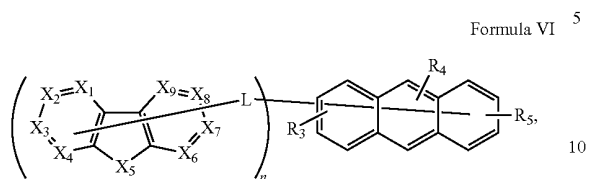


wherein  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  may represent mono, di, tri, or tetra substitutions; and

wherein  $R_3$ ,  $R_4$ ,  $R_5$  and  $R_6$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, and aryl.

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20. The device of claim 14, wherein the compound has the formula:

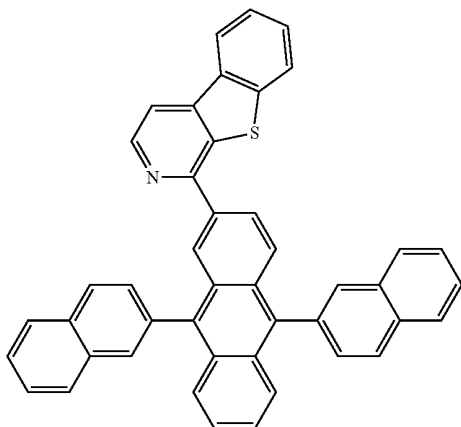


wherein  $R_3$ ,  $R_4$ , and  $R_5$  may represent mono, di, tri, or tetra substitutions; and

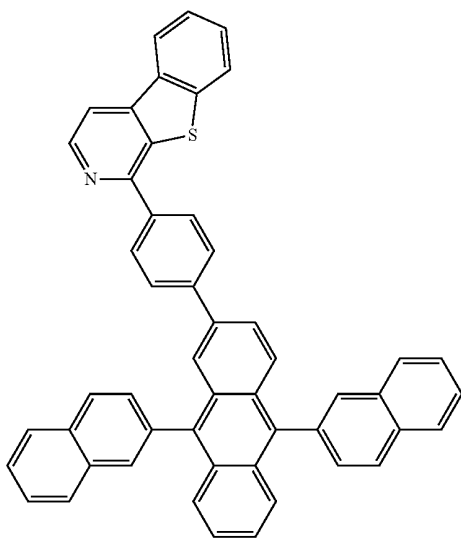
wherein  $R_3$ ,  $R_4$ , and  $R_5$  are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, silyl, cyano, halogen, aryl, and heteroaryl.

21. The first device of claim 14, wherein the compound is selected from the group consisting of:

Compound 1



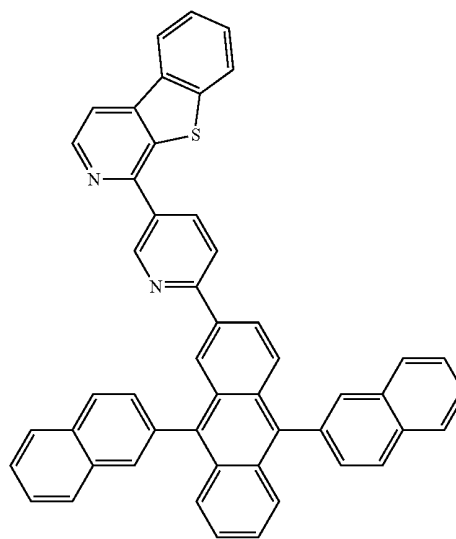
Compound 2



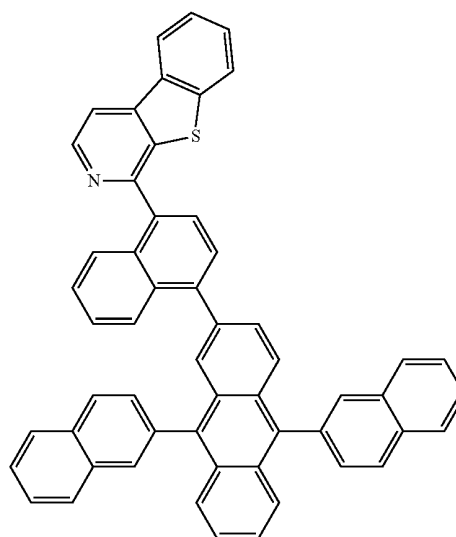
174

-continued

Compound 3

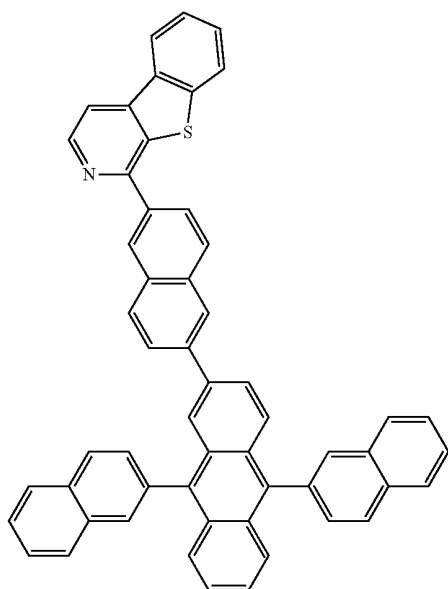


Compound 4



**175**

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Compound 5

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Compound 6

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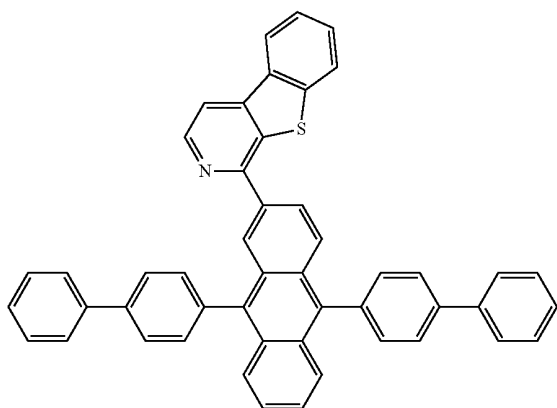
Compound 7

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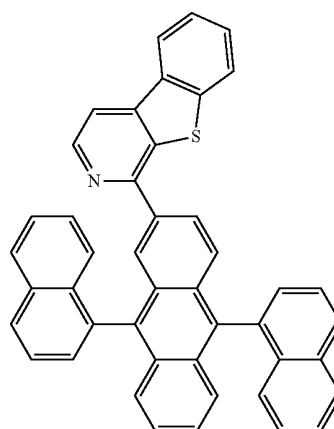
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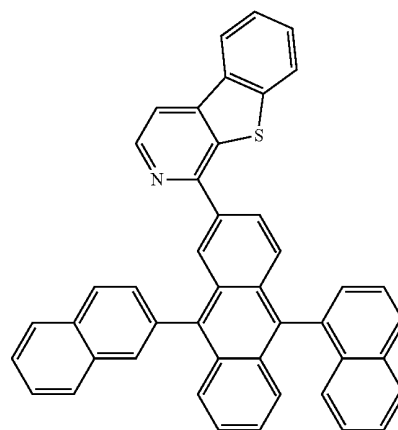
65

**176**

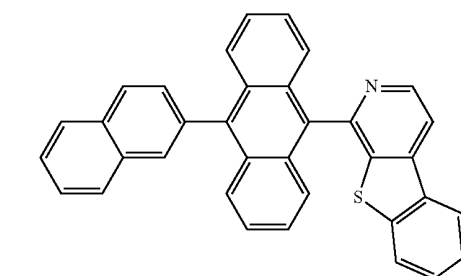
-continued



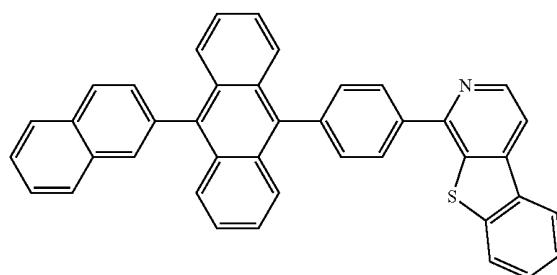
Compound 8



Compound 9

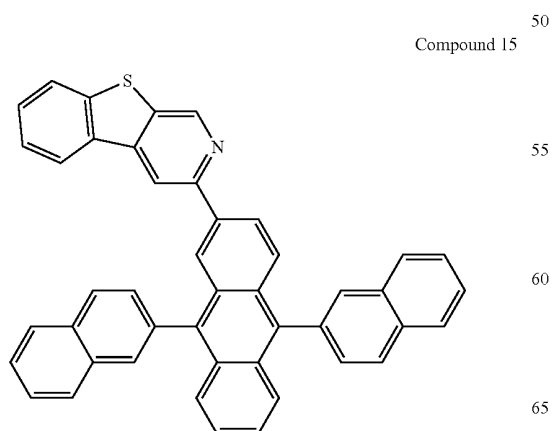
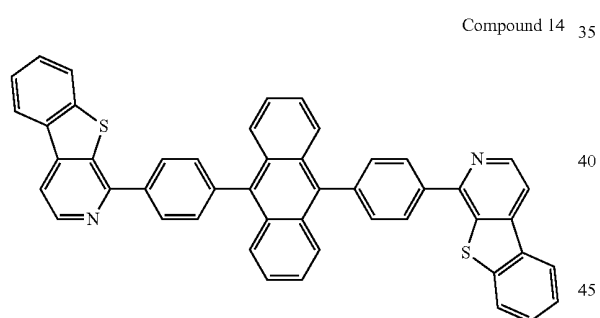
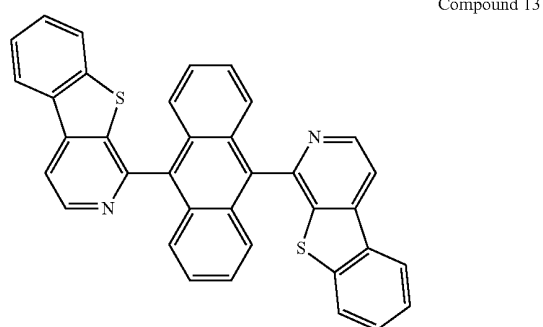
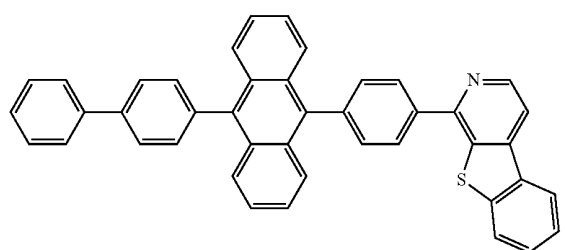


Compound 10

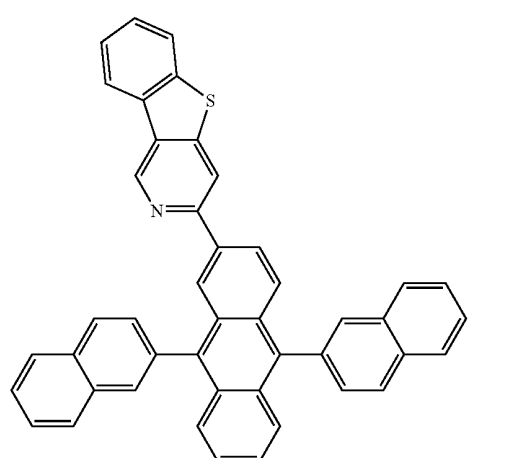
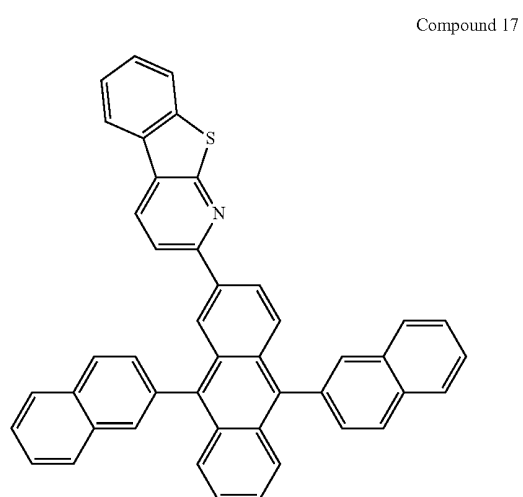
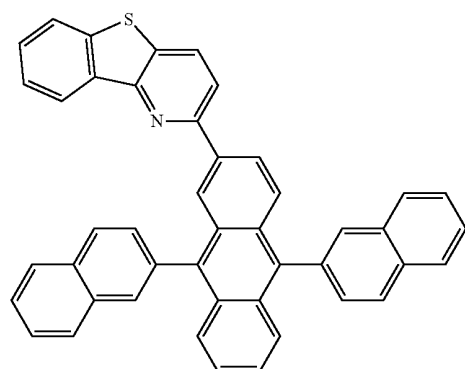


Compound 11

**177**  
-continued

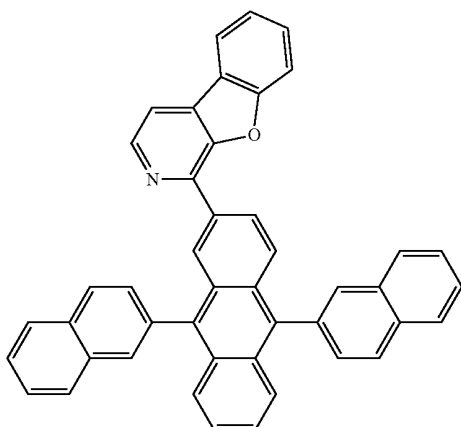


**178**  
-continued

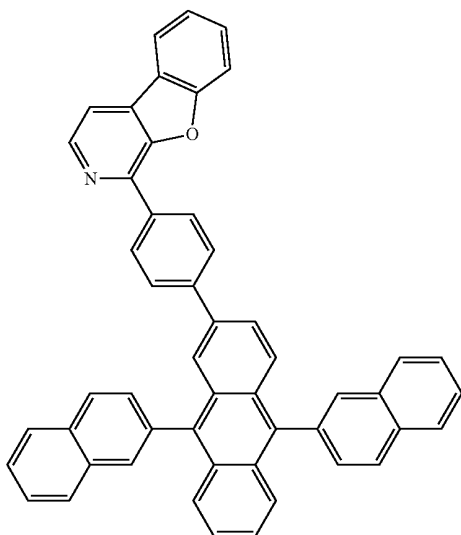


**179**  
-continued

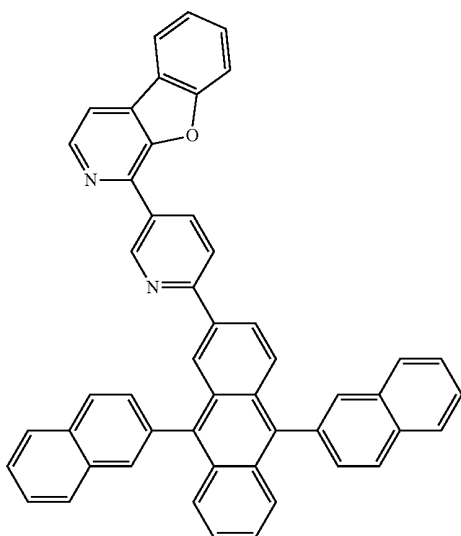
Compound 19



Compound 20

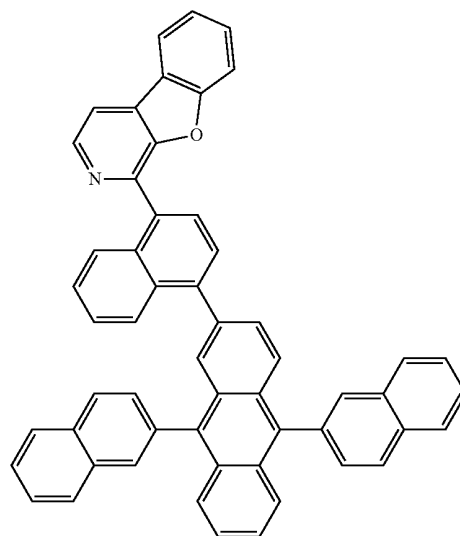


Compound 21

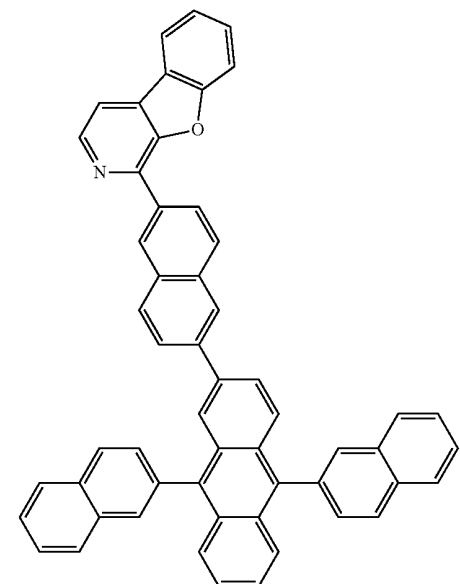


**180**  
-continued

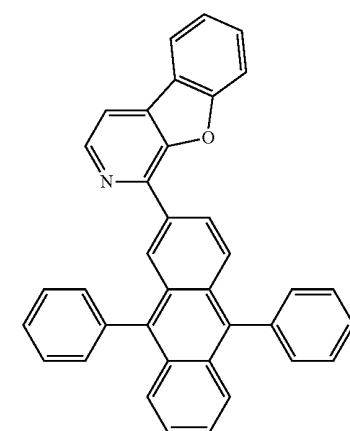
Compound 22



Compound 23



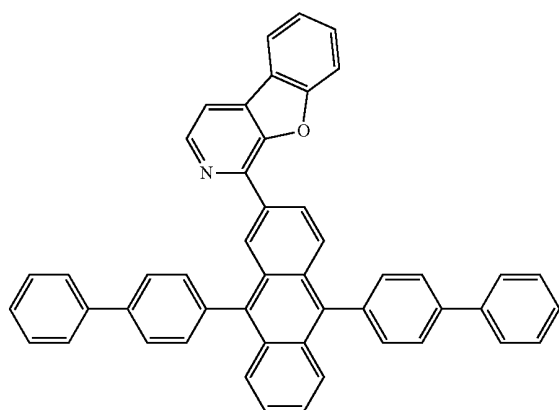
Compound 24



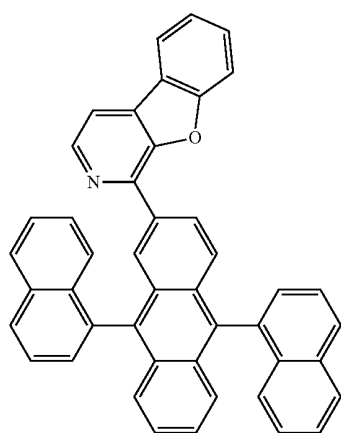


**181**

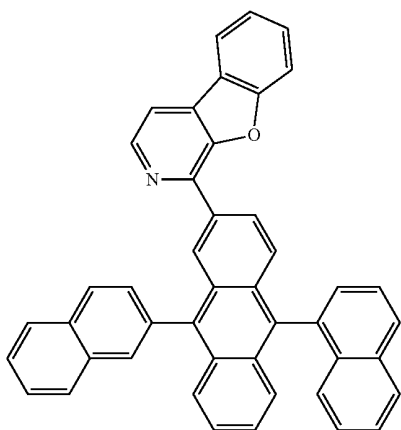
-continued



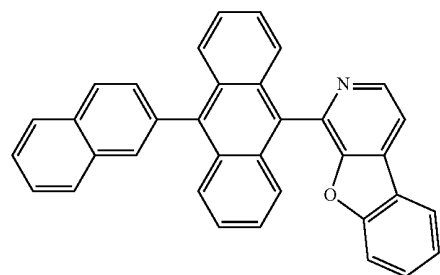
Compound 25



Compound 26



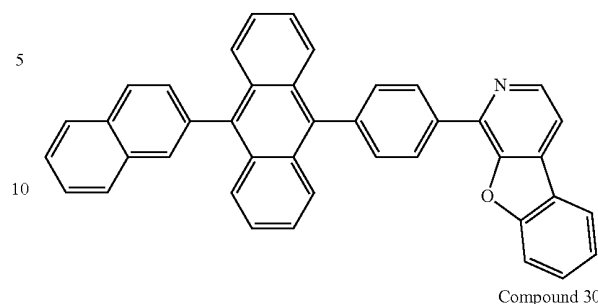
Compound 27



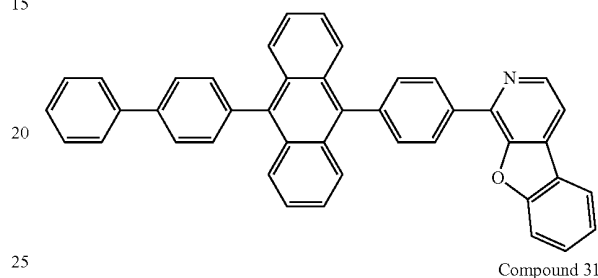
Compound 28

**182**

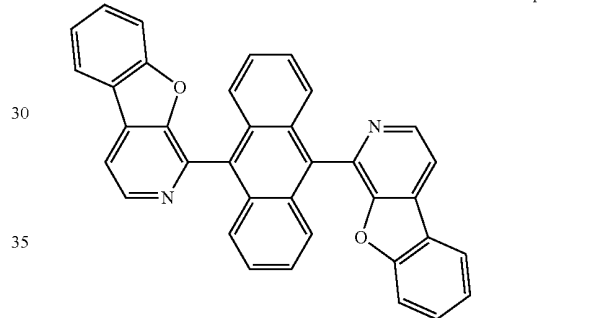
-continued



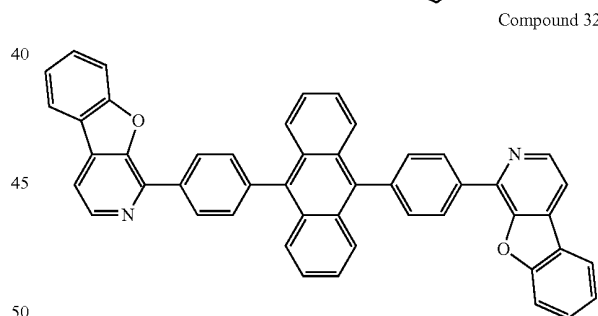
Compound 29



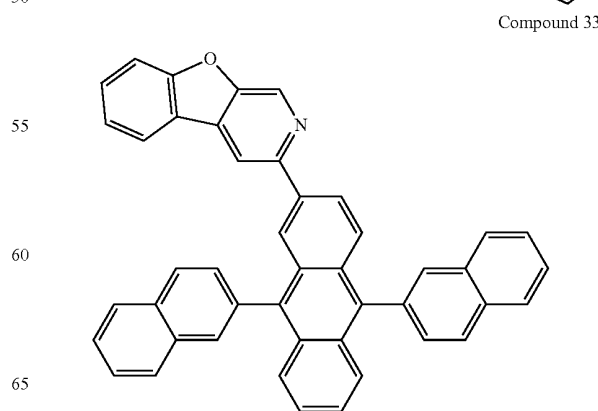
Compound 30



Compound 31



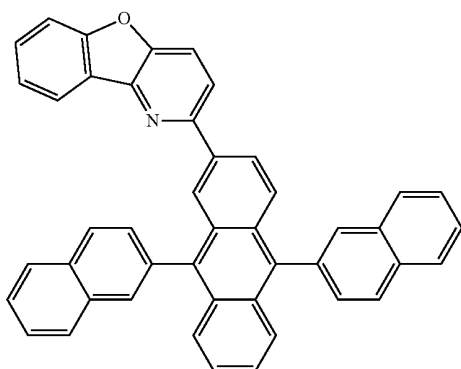
Compound 32



Compound 33

**183**  
-continued

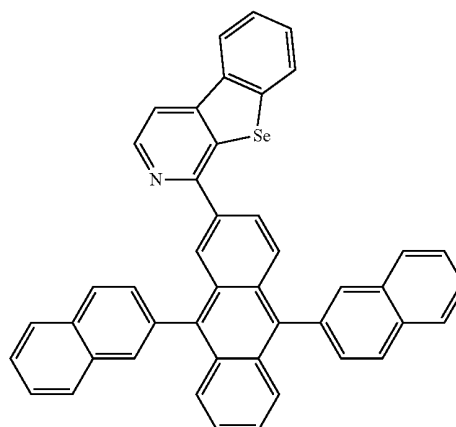
Compound 34



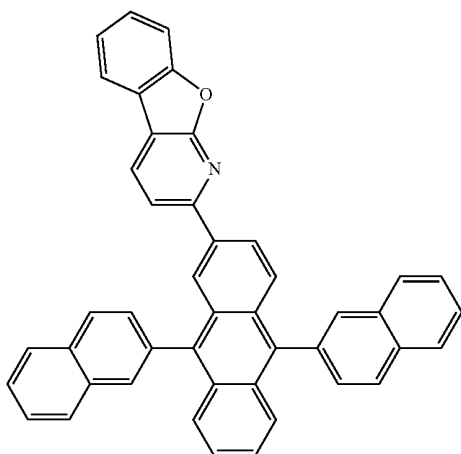
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**184**  
-continued

Compound 37

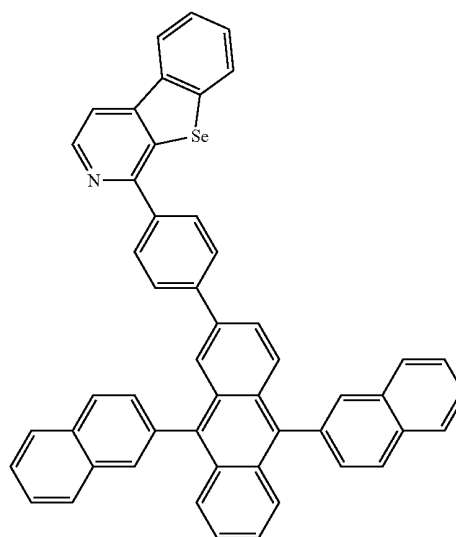


Compound 35

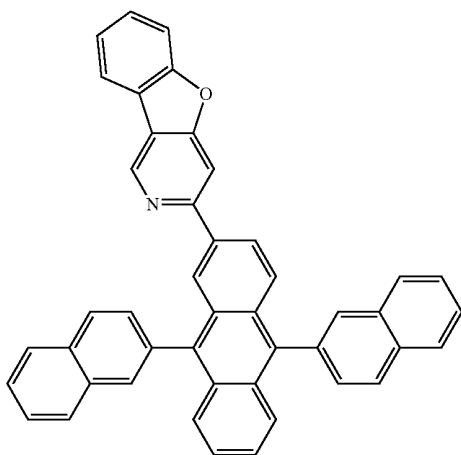


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Compound 38

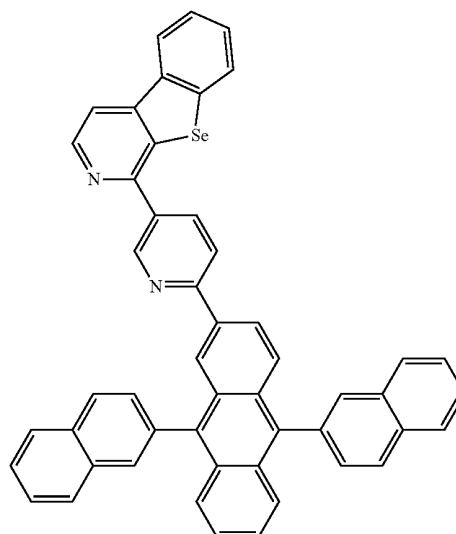


Compound 36



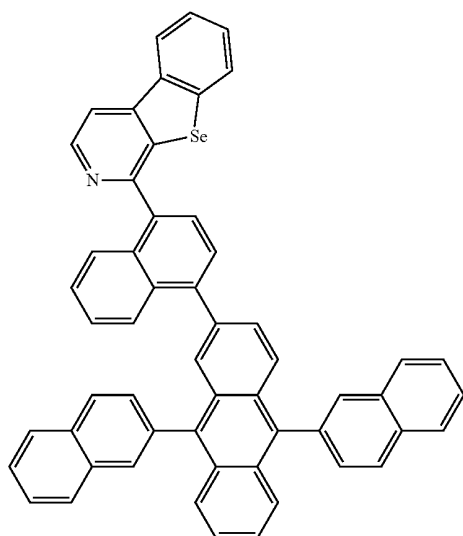
50  
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Compound 39



**185**

-continued



Compound 40

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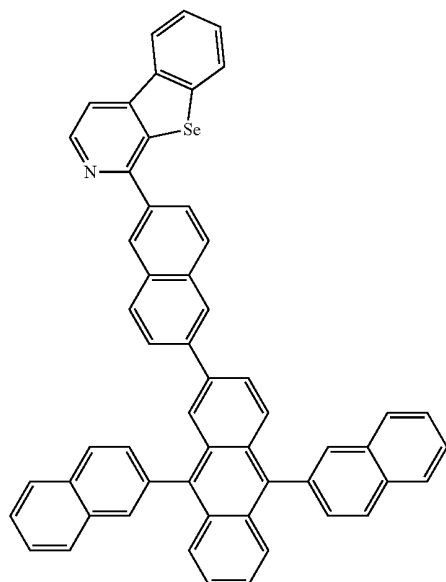
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Compound 41

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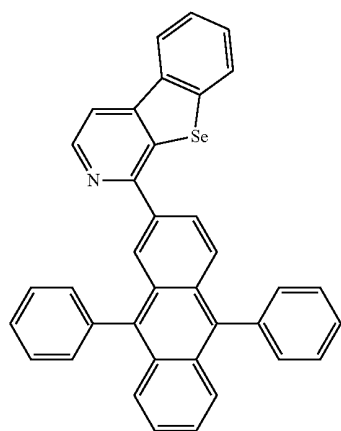


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Compound 42

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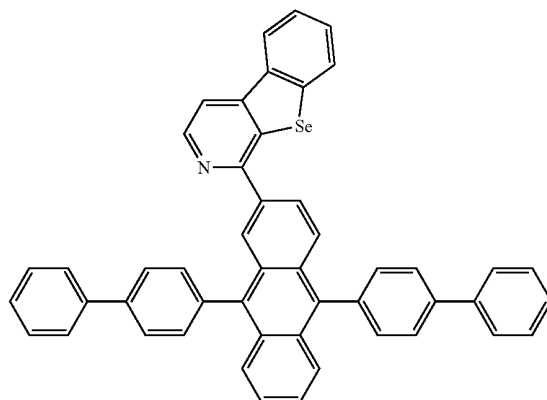
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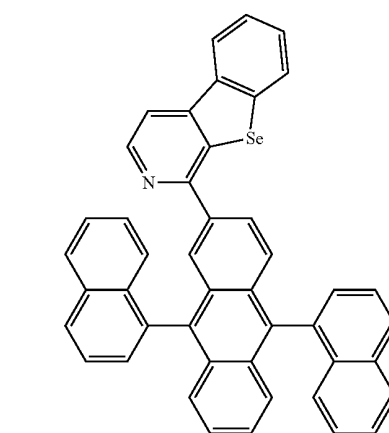
**186**

-continued

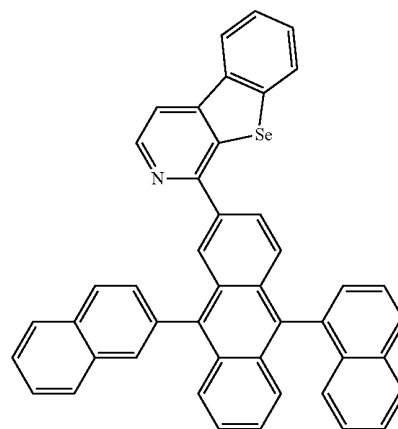


Compound 43

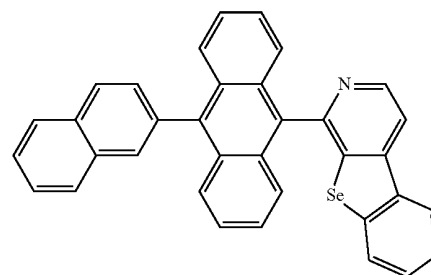
Compound 44



Compound 45



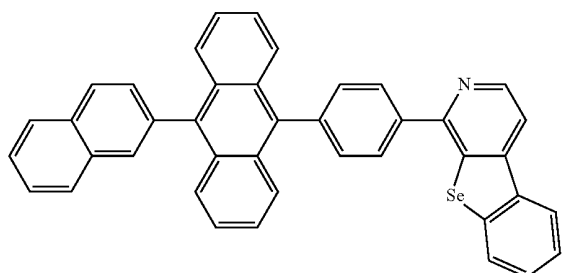
Compound 46



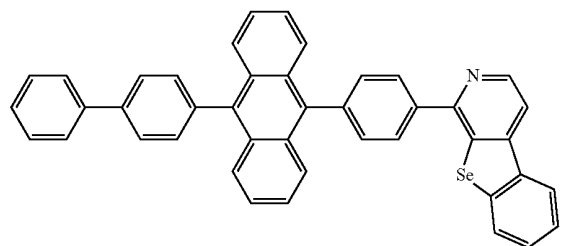
**187**

-continued

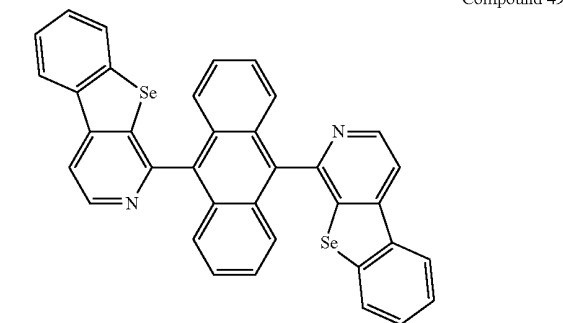
Compound 47



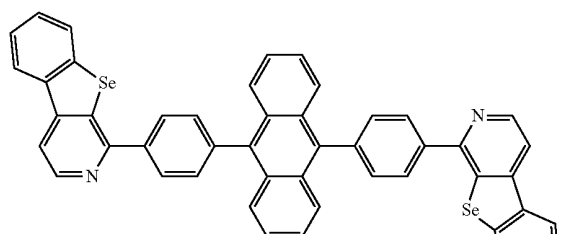
Compound 48



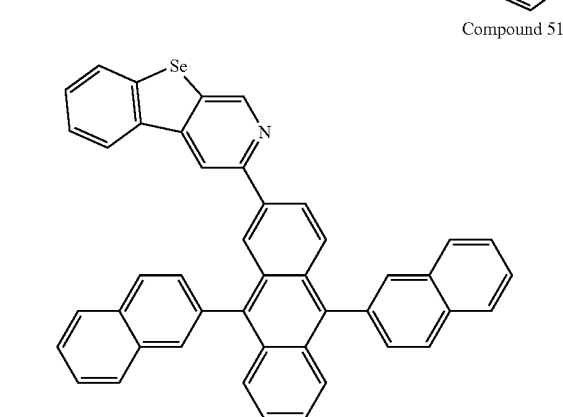
Compound 49



Compound 50

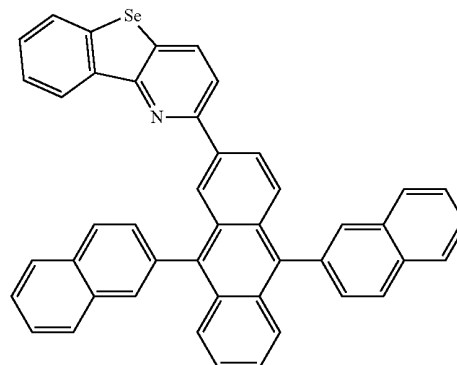


Compound 51

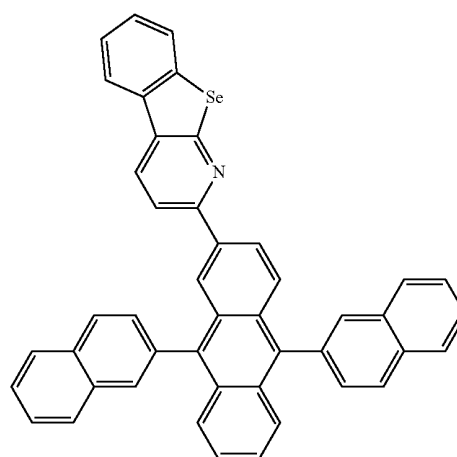
**188**

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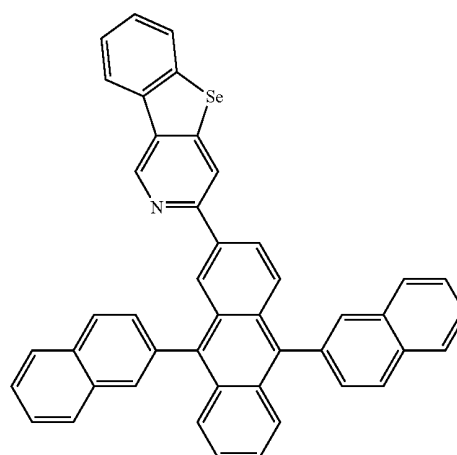
Compound 52

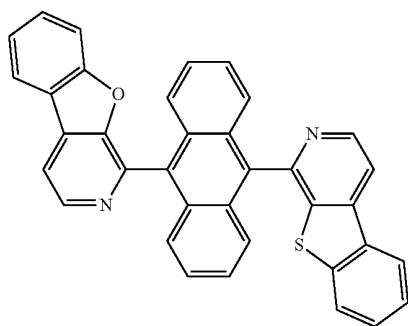


Compound 53



Compound 54



**189**  
-continued

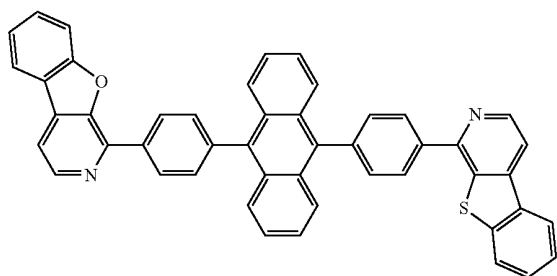
Compound 55

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Compound 56

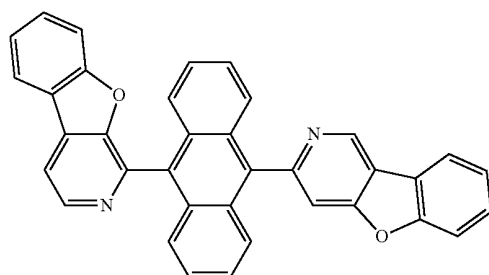


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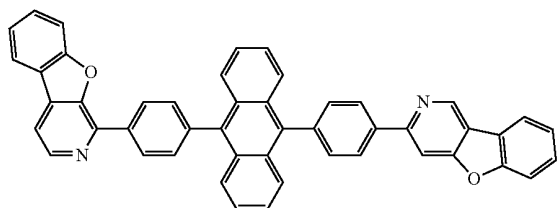
Compound 57



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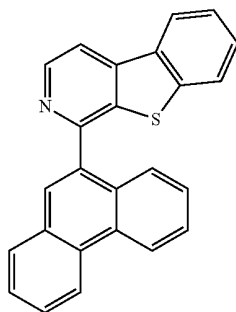
Compound 58



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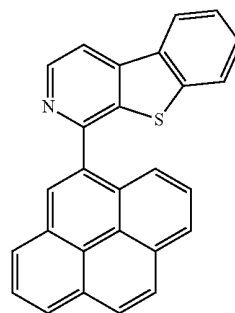
Compound 59



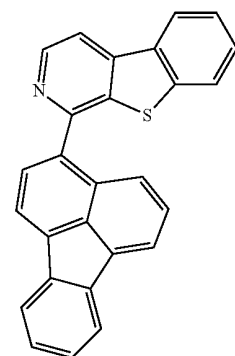
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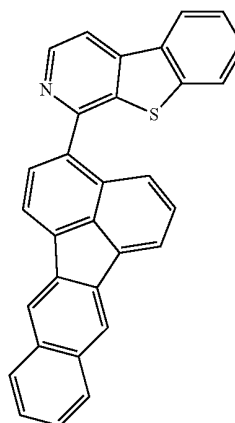
65

**190**  
-continued

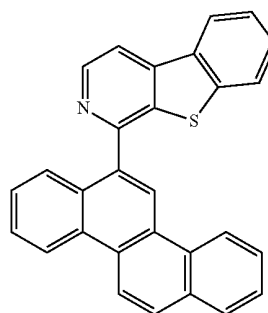
Compound 60



Compound 61



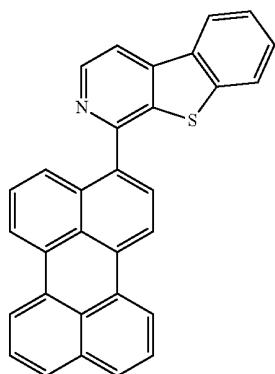
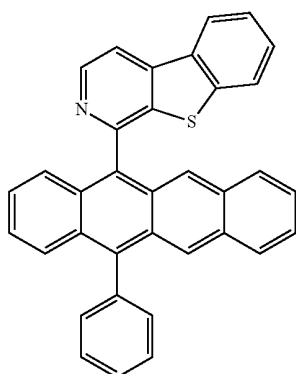
Compound 62



Compound 63

**191**

-continued



22. The first device of claim 14, wherein the organic layer is a non-emissive layer and the compound is a non-emissive compound.

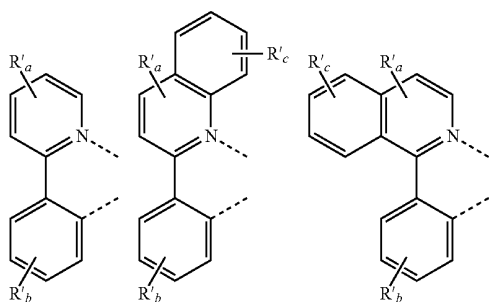
23. The first device of claim 22, wherein the organic layer is an electron transport layer and the compound is an electron transport material.

24. The first device of claim 23, wherein the electron transport layer is doped with an n-type conductivity dopant.

25. The first device of claim 24, wherein the n-type conductivity dopant is a compound containing Li, Na, K, Rb, or Cs.

26. The first device of claim 25, wherein the n-type conductivity dopant is selected from the group consisting of LiF, CsF, NaCl, KBr, and LiQ.

27. The first device of claim 14, wherein the organic layer further comprises an emissive compound that is a transition metal complex having at least one ligand selected from the group consisting of:



Compound 64

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15

Compound 65

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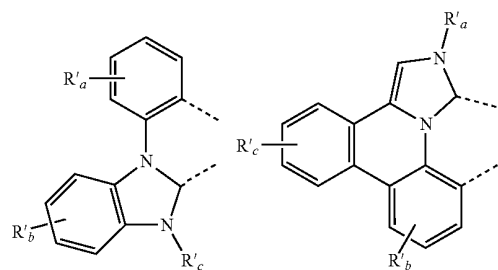
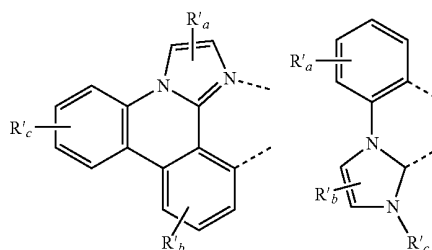
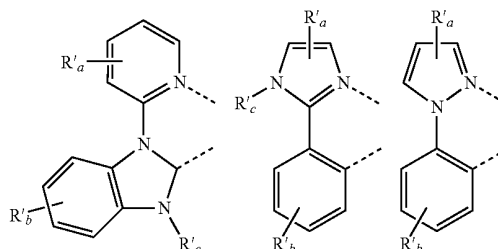
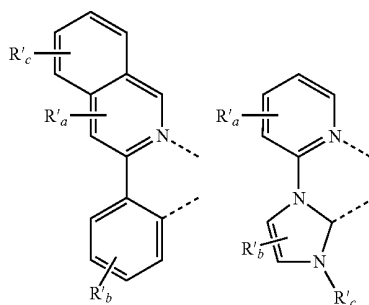
45

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**192**

-continued



wherein each of  $R'_a$ ,  $R'_b$  and  $R'_c$  may represent mono, di, tri, or tetra substituents;

wherein each of  $R'_a$ ,  $R'_b$  and  $R'_c$  are independently selected from a group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, or heteroaryl; and

wherein two adjacent substituents may form into a ring.

28. The first device of claim 14, wherein the first device is a consumer product.

29. The first device of claim 14, wherein the first device is an organic light emitting device.

\* \* \* \* \*

专利名称(译)	电子传输化合物		
公开(公告)号	<a href="#">US8415031</a>	公开(公告)日	2013-04-09
申请号	US13/012425	申请日	2011-01-24
[标]申请(专利权)人(译)	环球展览公司		
申请(专利权)人(译)	通用显示器公司		
当前申请(专利权)人(译)	通用显示器公司		
[标]发明人	XIA CHUANJUN MOHAN SIDDHARTH HARIKRISHNA ADAMOVICH VADIM		
发明人	XIA, CHUANJUN MOHAN, SIDDHARTH HARIKRISHNA ADAMOVICH, VADIM		
IPC分类号	H01L51/54		
CPC分类号	C07D491/04 C07D495/04 C07D517/04 H01L51/0058 H01L51/5072		
代理机构(译)	KILPATRICK TOWNSEND & STOCKTON LLP		
助理审查员(译)	CLARK , GREGORY		
其他公开文献	US20120187381A1		
外部链接	<a href="#">Espacenet</a> <a href="#">USPTO</a>		

#### 摘要(译)

提供了包含氮杂 - 二苯并部分和具有至少三个苯环的稠合芳族部分的化合物。特别地，所述化合物可包含直接或间接与蒽连接的氮杂二苯并呋喃，氮杂二苯并噻吩或氮杂二苯并硒吩。该化合物可用于有机发光器件的电子传输层中，以提供具有改进性能的器件。

