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(54) BICARBAZOLE COMPOUNDS FOR OLEDS

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(57) ABSTRACT

Novel organic compounds comprising a bicarbazole core are provided. In particular, the compounds has a 3,3'-bicarbazole core substituted at the 9-position with a triazine or pyrimidine. The compounds may be used in organic light emitting devices to provide devices having improved efficiency and improved lifetime.

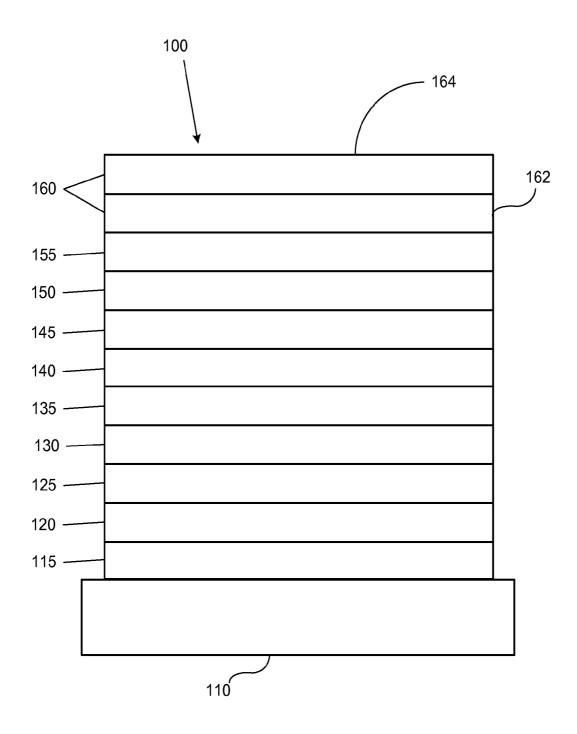


FIGURE 1

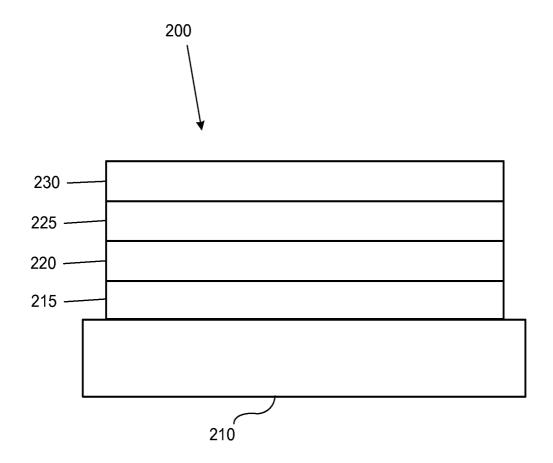


FIGURE 2

$$R_3$$
 R_4
 R_1
 R_2
 R_2
 R_4
 R_4
 R_4
 R_4
 R_4

FIGURE 3

BICARBAZOLE COMPOUNDS FOR OLEDS

[0001] 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

[0002] The present invention relates to organic light emitting devices (OLEDs). More specifically, the present invention pertains to phosphorescent organic materials comprising a bicarbazole having a nitrogen-containing heterocycle at the 9 position.

BACKGROUND

[0003] 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.

[0004] 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.

[0005] 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.

[0006] One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)₃, which has the structure:

[0007] In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

[0008] 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.

[0009] 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.

[0010] 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.

[0011] 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.

[0012] 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.

[0013] 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.

[0014] 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

[0015] Compounds comprising a bicarbazole are provided. The compounds have the formula:

Formula I

$$R_1$$
 R_2
 R_2
 R_2
 R_3
 R_4
 R_4

[0016] R₁, R₂, R₃, and R₄ may represent mono, di, tri, or tetra substitutions. R₁, R₂, R₃, and R₄ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl. Ar_1 , Ar_2 , and Ar_3 are independently selected from aryl or heteroaryl. Ar_1 , Ar_2 , and Ar_3 may be further substituted. X is C or N.

[0017] In one aspect, Ar_1 , Ar_2 , and Ar_3 are independently selected from the group consisting of phenyl, pyridine, naphthalene, biphenyl, terphenyl, fluorene, dibenzofuran, dibenzothiophene, phenanthrene, and triphenylene. Ar_1 , Ar_2 , and Ar_3 are independently further substituted with a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl, but the substituent is not an aryl or heteroaryl fused directly to Ar_1 , Ar_2 , and Ar_3 . Preferably, Ar_1 and Ar_2 are independently selected from the group consisting of phenyl, pyridine, and naphthalene. Preferably, Ar_3 is selected from the group consisting of phenyl, biphenyl, dibenzofuran, and dibenzothiophene.

[0018] In another aspect, R_1 , R_2 , R_3 , and R_4 are hydrogen.

[0019] Specific examples of compounds comprising bicarbazole are also provided. In particular, the compound is selected from the group consisting of:

Compound 1

Compound 3

Compound 7

Compound 11

Compound 15

Compound 19

Compound 25

Compound 31

-continued -continued

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Compound 43

-continued -continued

Compound 48

Compound 51

Compound 55

Compound 59

-continued -continued

Compound 63

Compound 67

Compound 71

Compound 75

Compound 78

Compound 83

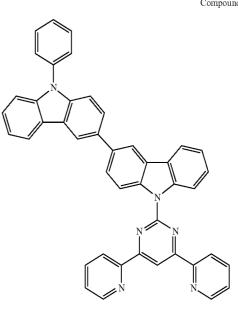
Compound 87

-continued -continued

-continued -continued

Compound 103

Compound 104



Compound 107

0 1100

Compound 111

-continued -continued

-continued -continued

Compound 119

-continued -continued

Compound 127

Compound 131

Compound 135

Compound 139

-continued -continued

Compound 147

Compound 150

Compound 151

-continued -continued

Compound 163

Compound 167

-continued -continued

Compound 171

-continued -continued

Compound 175

-continued

[0027] In another aspect, the organic layer further comprises an emissive dopant having the formula:

[0020] A first device comprising an organic light emitting device is also provided. The device further comprises an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprises a compound having Formula I, as described above.

[0021] R₁, R₂, R₃, and R₄ may represent mono, di, tri, or tetra substitutions. R₁, R₂, R₃, and R₄ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl. Ar_1 , Ar_2 , and Ar_3 are independently selected from aryl or heteroaryl. Ar_1 , Ar_2 , and Ar_3 may be further substituted. X is C or N.

[0022] In one aspect, Ar₁, Ar₂, and Ar₃ are independently selected from the group consisting of phenyl, pyridine, naphthalene, biphenyl, terphenyl, fluorene, dibenzofuran, dibenzothiophene, phenanthrene, and triphenylene. Ar₁, Ar₂, and Ar₃ are independently further substituted with a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl, but the substituent is not an aryl or heteroaryl fused directly to Ar₁, Ar₂, and Ar₃. Preferably, Ar₁ and Ar₂ are independently selected from the group consisting of phenyl, pyridine, and naphthalene. Preferably, Ar₃ is selected from the group consisting of phenyl, biphenyl, dibenzofuran, and dibenzothiophene.

[0023] In another aspect, R_1 , R_2 , R_3 , and R_4 are hydrogen.

[0024] Specific examples of devices containing compounds comprising bicarbazole are also provided. In particular, the compound is selected from the group consisting of Compound 1-Compound 184.

[0025] In one aspect, the organic layer is deposited using solution processing.

[0026] In one aspect, the organic layer is an emissive layer and the compound having Formula I is a host.

D10

D18

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

D37

D43

D44

D45

D46

D47

-continued

[0028] 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

[0030] FIG. 1 shows an organic light emitting device.
[0030] FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.
[0031] FIG. 3 shows a bicarbazole compound with a nitrogen-containing heterocycle substitution at the 9-position.

DETAILED DESCRIPTION

[0032] 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.

[0033] 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. [0034] 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.

[0035] 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.

[0036] 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, electricallyconductive, 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

[0037] 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. [0038] 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. [0039] 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 outcoupling, 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.

[0040] 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.

[0041] 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.).

[0042] 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.

[0043] 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.

[0044] Novel bicarbazole containing compounds are provided (illustrated in FIG. 3). More specifically, these compounds contain a 3,3'-bicarbazole core and triazine or pyrimidine substitution at the 9-position. These compounds may be used as hosts for phosphorescent OLEDs.

[0045] Carbazole containing compounds for use as OLED materials have been previously described. In particular, 3,3'-bicarbazole compounds have good hole transporting properties, but have poor stability toward electrons. Alkyl and aryl substituted 3,3'-bicarbazole compounds have been used as hole transporting materials and hosts in OLEDs; however, these compounds also have imbalanced charge transporting properties and poor electron stability and may provide devices with low efficiency and limited lifetime. For example, a diaryl substituted 3,3'-bicarbazole, i.e. H1, has a HOMO around 5.6 eV, very good for hole transporting but poor for electron transporting and stability. Therefore, the 3,3'-bicarbazole compounds reported in the literature may have limited use.

[0046] In the present invention, nitrogen containing electron deficient heterocycles were introduced to 3,3'-bicarbazole compounds. In particular, the compounds contain a 3,3'-bicarbazole core and triazine or pyrimidine substitution at the 9 position. The nitrogen containing heterocycle tunes the HOMO/LUMO levels as well as increases the compound's stability toward electrons. In addition, these compounds contain a donor part, i.e. bicarbazole, and an acceptor part, i.e. electron deficient nitrogen heterocycle. Without being bound by theory, it is believed that these donor-acceptor type molecules can shrink singlet and triplet gap and improve stability to both hole and electrons. Therefore, these 3,3'-bicarbazole compounds containing a nitrogen heterocycle may provide devices having better stability and lower operating voltage.

[0047] Compounds comprising a bicarbazole are provided. The compounds have the formula:

Formula I

$$R_1$$
 R_2
 R_2
 R_4
 R_4
 R_4

[0048] R₁, R₂, R₃, and R₄ may represent mono, di, tri, or tetra substitutions. R₁, R₂, R₃, and R₄ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl. Ar₁, Ar₂, and Ar₃ are independently selected from aryl or heteroaryl. Ar₁, Ar₂, and Ar₃ may be further substituted. X is C or N.

[0049] In one aspect, Ar_1 , Ar_2 , and Ar_3 are independently selected from the group consisting of phenyl, pyridine, naphthalene, biphenyl, terphenyl, fluorene, dibenzofuran, dibenzothiophene, phenanthrene, and triphenylene, and Ar_1 , Ar_2 , and Ar_3 are independently further substituted with a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl, but the substituent is not an aryl or heteroaryl fused directly to Ar_1 , Ar_2 , and Ar_3 . Preferably, Ar_1 and Ar_2 are independently selected from the group consisting of phenyl, pyridine, and naphthalene. Preferably, Ar_3 is selected from the group consisting of phenyl, biphenyl, dibenzofuran, and dibenzothiophene.

[0050] In another aspect, R_1 , R_2 , R_3 , and R_4 are hydrogen. [0051] Specific examples of compounds comprising bicarbazole are also provided. In particular, the compound is selected from the group consisting of:

-continued -continued

Compound 3

-continued -continued

-continued -continued

Compound 23

-continued -continued

Compound 47

Compound 51

Compound 55

Compound 59

Compound 66

-continued -continued

Compound 64

Compound 67

Compound 71

-continued -continued

Compound 79

Compound 86

-continued -continued

Compound 102

-continued -continued

Compound 103

Compound 106

Compound 107

-continued -continued

Compound 115

Compound 122

-continued -continued

Compound 135

-continued -continued

-continued -continued

Compound 147

-continued -continued

Compound 151

Compound 154

Compound 155

Compound 156

d 156 Compound 158

-continued -continued

Compound 159

Compound 163

-continued -continued

-continued -continued

Compound 171

Compound 172

Compound 175

Compound 179

Compound 180

Compound 183

[0052] A first device comprising an organic light emitting device is also provided. The device further comprises an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprises a compound having Formula I, as described above.

[0053] R₁, R₂, R₃, and R₄ may represent mono, di, tri, or tetra substitutions. R₁, R₂, R₃, and R₄ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl. Ar₁, Ar₂, and Ar₃ are independently selected from aryl or heteroaryl. Ar₁, Ar₂, and Ar₃ may be further substituted. X is C or N.

[0054] In one aspect, Ar_1 , Ar_2 , and Ar_3 are independently selected from the group consisting of phenyl, pyridine, naphthalene, biphenyl, terphenyl, fluorene, dibenzofuran, dibenzothiophene, phenanthrene, and triphenylene. Ar_1 , Ar_2 , and Ar_3 are independently further substituted with a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl, but the substituent is not an aryl or heteroaryl fused directly to Ar_1 , Ar_2 , and

 Ar_3 . Preferably, Ar_1 and Ar_2 are independently selected from the group consisting of phenyl, pyridine, and naphthalene. Preferably, Ar_3 is selected from the group consisting of phenyl, biphenyl, dibenzofuran, and dibenzothiophene.

[0055] In another aspect, R_1 , R_2 , R_3 , and R_4 are hydrogen.

[0056] Specific examples of devices containing compounds comprising bicarbazole are also provided. In particular, the compound is selected from the group consisting of Compound 1-Compound 184.

[0057] In one aspect, the organic layer is deposited using solution processing.

[0058] In one aspect, the organic layer is an emissive layer and the compound having Formula I is a host.

[0059] In another aspect, the organic layer further comprises an emissive dopant having the formula:

-continued

D18

-continued

-continued

-continued

$$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_2$$

-continued

D42

-continued

D43

D44

D45

D46

[0060] 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

[0061] 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:

[0062] A hole injecting/transporting material to be used in 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 not limit to: a phthalocyanine or porphryin 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 sliane derivatives; a metal oxide derivative, such as MoO_x ; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

[0063] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:

$$Ar^{2} \xrightarrow{Ar^{3}} Ar^{3} \xrightarrow{Ar^{3}} Ar^{3} \xrightarrow{Ar^{4}} Ar^{4} \xrightarrow{Ar^{4}} Ar^{4} \xrightarrow{Ar^{5}} Ar^{7}$$

$$Ar^{2} \xrightarrow{Ar^{3}} Ar^{3} \xrightarrow{Ar^{5}} Ar^{5} \xrightarrow{Ar^{5}} Ar^{5}$$

-continued

$$Ar^{4}$$

$$N - Ar^{1} - N$$

$$Ar^{5}$$

$$Ar^{6} - N$$

$$Ar^{7}$$

$$Ar^{8}$$

$$Ar^{9}$$

$$Ar^{9}$$

$$Ar^{9}$$

$$Ar^{7}$$

$$Ar^{7}$$

$$Ar^{8}$$

$$Ar^{8}$$

[0064] Each of Ar¹ to Ar⁹ is selected from the group consisting 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, pyrrolodipyridine, 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, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, 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 Ar is further substituted by a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

[0065] In one aspect, Ar¹ to Ar⁹ is independently selected from the group consisting of:

[0066] k is an integer from 1 to 20; X^1 to X^8 is CH or N; Ar^1 has the same group defined above.

[0067] Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:

$$\begin{bmatrix} \begin{pmatrix} Y^1 \\ Y^2 \end{pmatrix}_m M$$
—Ln

[0068] M is a metal, having an atomic weight greater than 40; (Y^1-Y^2) is a bidentate ligand, Y1 and Y^2 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. [0069] In one aspect, (Y^1-Y^2) is a 2-phenylpyridine deriva-

tive.

In another aspect, (Y¹-Y²) is a carbene ligand. [0070]

[0071] In another aspect, M is selected from Ir, Pt, Os, and

[0072] In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc+/Fc couple less than about 0.6 V.

Host:

[0073] The light emitting layer of the organic EL device 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.

[0074] Examples of metal complexes used as host are preferred to have the following general formula:

$$\begin{bmatrix} \begin{pmatrix} Y^3 \\ Y^4 \end{bmatrix}_m M - Ln \end{bmatrix}$$

[0075] M is a metal; (Y^3-Y^4) is a bidentate ligand, Y^3 and Y⁴ 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.

[0076] In one aspect, the metal complexes are:

$$\begin{bmatrix} O \\ N \end{bmatrix}_{m} Al - L_{3-m} \begin{bmatrix} O \\ N \end{bmatrix}_{m} Zn - L_{2-m}$$

[0077] (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

[0078] In another aspect, M is selected from Ir and Pt.

[0079] In a further aspect, (Y^3-Y^4) is a carbene ligand.

[0080] Examples of organic compounds used as host are selected from the group consisting 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, pyrrolodipyridine, 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, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, 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 substituted by a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

[0081] In one aspect, host compound contains at least one of the following groups in the molecule:

[0082] R^1 to R^7 is independently selected from the group consisting of hydrogen, 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.

[0083] k is an integer from 0 to 20.

[0084] X^1 to X^8 is selected from CH or N.

HBL:

[0085] 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.

[0086] In one aspect, compound used in HBL contains the same molecule used as host described above.

[0087] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

[0088] k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

ETL:

[0089] 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.

[0090] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

$$F$$
 F
 F

[0091] R¹ is selected from the group consisting of hydrogen, 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.

[0092] Ar^1 to Ar^3 has the similar definition as Ar's mentioned above.

[0093] k is an integer from 0 to 20.

[0094] X^1 to X^8 is selected from CH or N.

[0095] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

$$\begin{bmatrix} O \\ N \end{bmatrix}_{m} Al - L_{3-m} \begin{bmatrix} O \\ N \end{bmatrix}_{m} Be - L_{2-m} \begin{bmatrix} O \\ N \end{bmatrix}_{m} Zn - L_{2-m} \begin{bmatrix} N \\ N \end{bmatrix}_{m} Zn - L_{2-m} \begin{bmatrix} O \\ N \end{bmatrix}_{m} Zn -$$

[0096] (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.

[0097] In any above-mentioned compounds used in each layer of OLED device, the hydrogen atoms attached to conjugated rings can be partially or fully deuterated.

[0098] 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.

[0099] In addition to and/or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Nonlimiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 1 below. Table 1 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 1

	TABLE 1	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and pomphryin compounds	N Cu N	Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF _x Fluorohydrocarbon polymer	$ CH_xF_y$ $\frac{1}{n}$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)	$+$ SO_3 (H^+) R	Synth. Met. 87, 171 (1997) WO2007002683

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phosphonic acid and sliane SAMs	N — $SiCl_3$	US20030162053
Triarylamine or polythiophene polymers with conductivity dopants		EA01725079A1
	Br N +N	
	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
Arylamines complexed with metal oxides such as molybdenum and tungsten oxides	+ MoC	SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 1-continued

TABLE 1-continued		
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
p-type semiconducting organic complexes	NC CN N N N CN NC CN NC CN	US20020158242
Metal organometallic complexes	Ir 3	US20060240279
Cross-linkable compounds		US20080220265
Trianglandon	Hole transporting materials	Anal Dhon Lot
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 5,061,569
		EP650955
		J. Mater. Chem. 3, 319 (1993)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)

Triaylamine on spirofluorene core

$$\begin{array}{c} Ph_2N \\ \\ Ph_2N \\ \end{array}$$

$$\begin{array}{c} NPh_2 \\ \\ NPh_2 \\ \end{array}$$

Synth. Met. 91, 209 (1997)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190
Indolocarbazoles		Synth. Met. 111, 421 (2000)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Isoindole compounds	EAGULES OF MATERIAL	Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Arylcarbazoles	Phosphorescent OLED host materials Red hosts	Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq ₃ , BAlq)	N N AI	Nature 395, 151 (1998)
	$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix} \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix} \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix} \begin{bmatrix} \\ \\ \\ \\$	US20060202194

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Al-O	WO2005014551
	$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{0} \end{bmatrix}_{2} A I - O - \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{0} $	WO2006072002
Metal phenoxybenzothiazole compounds	S N Zn	Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)	$C_{8}H_{17}$ $C_{8}H_{17}$	Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045730, US20090045731, WO2009008311, US20090008605, US20090009065
Zinc complexes	H N Zn N H	WO2009062578

TABLE 1-continued

TABLE 1-continued		
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Green hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
	N N N N N N N N N N N N N N N N N N N	US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965
		US20060280965

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2009021126
Donor acceptor type molecules		WO2008056746
Aza-carbazole/		JP2008074939
DBT/DBF		N
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207

TABLE 1-continued		
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal phenoxybenzooxazole compounds	Al—O—	WO2005089025
	ON AI ON N	WO2006132173
	Zn 2	JP200511610
Spirofluorene-carbazole compounds		JP2007254297

TABLE 1-continued

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

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds	Zn O 2	WO2005030900
Metal coordination complexes (e.g., Zn, Al with NAN ligands)	N N N Zn	US20040137268, US20040137267
Arylcarbazoles	Blue hosts	Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzothiophene/ Dibenzofuran-carbazole compounds	N N N N N N N N N N N N N N N N N N N	WO2006114966, US20090167162
		US20090167162
		WO2009086028
	S S S S S S S S S S S S S S S S S S S	US20090030202, US20090017330
Silicon aryl compounds		US20050238919

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	S _{Si} S _{Si}	WO2009003898
Silicon/Germanium aryl compounds	S _{Si}	EP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex	Phosphorescent dopants Red dopants	U.S. Pat. No. 7,154,114
Heavy metal porphyrins (e.g., PtOEP)	$\begin{array}{c} Et \\ \\ \\ Et \\ \\ \\ Et \\ \\ \\ Et \\ \\ \\ Et \\ \\ \\ Et \\ \\ \\ Et \\ \\ Et \\ \\ \\ Et \\ \\ \\ \\$	Nature 395, 151 (1998)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Iridium(III) organometallic complexes	Ir O	Appl. Phys. Lett. 78, 1622 (2001)
	Ir o	US2006835469
		US2006835469
	Ir O	US20060202194
		US20060202194

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ir	US20070087321
	Ir	US20070087321
	$\operatorname{Ir}_{\operatorname{H}_{17}\operatorname{C}_{8}}$	Adv. Mater. 19, 739 (2007)
	Ir(acac)	WO2009100991
		WO2008101842

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Platinum(II) organometallic complexes	Pt O	WO2003040257
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes	$\begin{bmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & $	Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes	Re—(CO) ₄ Green dopants	US20050244673
Iridium(III) organometallic complexes	and its derivatives	Inorg. Chem. 40, 1704 (2001)

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20020034656
		U.S. Pat. No. 7,332,232
		US20090108737
	Ir	US20090039776

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ir S	U.S. Pat. No. 6,921,915
		U.S. Pat. No. 6,687,266
	Ir	Chem. Mater. 16, 2480 (2004)
	Ir	US20070190359
	Ir	US20060008670 JP2007123392

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ir o	Adv. Mater. 16, 2003 (2004)
	Ir N	Angew. Chem. Int. Ed. 2006, 45, 7800
	Ir	WO2009050290
	$\begin{bmatrix} \\ \\ \\ \end{bmatrix}_3$	US20090165846
		US20080015355

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Monomer for polymeric metal organometallic compounds	EXAMPLES OF MATERIAL O 1 1 2	U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentated ligands	N Pt—Cl	Appl. Phys. Lett. 86, 153505 (2005)
	Pt-O	Appl. Phys. Lett. 86, 153505 (2005)
	N Pt Fs	Chem. Lett. 34, 592 (2005)
	N Pt O	WO2002015645

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ph Pt N	US20060263635
Cu complexes	P Cu N N N	WO2009000673
Gold complexes	N—Au—N	Chem. Commun. 2906 (2005)
Rhenium(III) complexes	F ₃ C OC Re CO	Inorg. Chem. 42, 1248 (2003)

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Deuterated organometallic complexes	D D D Ir	US20030138657
Organometallic complexes with two or more metal centers		US20030152802
	F F S Blue dopants	U.S. Pat. No. 7,090,928
Iridium(III) organometallic complexes		WO2002002714

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ir 3	WO2006009024
	Ir	US20060251923
	Ir	U.S. Pat. No. 7,393,599, WO2006056418, US20050260441, WO2005019373
	Ir N	U.S. Pat. No. 7,534,505
	Ir ⁺	U.S. Pat. No. 7,445,855
	Ir	US20070190359, US20080297033

TABLE 1-continued

TABLE 1-continued		
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ir	U.S. Pat. No. 7,338,722
	N N N Ir	US20020134984
	N N N N N N N N N N N N N N N N N N N	Angew. Chem. Int. Ed. 47, 1 (2008)
	N Ir	Chem. Mater. 18, 5119 (2006)
	Ir F	Inorg. Chem. 46, 4308 (2007)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Ir	WO2005123873
	N Ir	WO2005123873
	Ir N Ir	WO2007004380
		WO2006082742
Osmium(II) complexes	Os N N 2	U.S. Pat. No. 7,279,704

TABLE 1-continued

TABLE 1-continued		
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	$\bigcap_{N} \bigcap_{N} \operatorname{Os}(PPh_3)$	Organometallics 23, 3745 (2004)
Gold complexes	Ph ₂ P PPh ₂ Au Au Cl	Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes	S N N N N N N N N N N N N N N N N N N N	WO2006098120, WO2006103874
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)	$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}$ $\begin{bmatrix} \\ $	Appl. Phys. Lett. 81, 162 (2002)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Appl. Phys. Lett. 79, 156 (2001)

TABLE 1-continued		
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085 O
	Electron transporting materials	
Anthracene- benzoimidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives	N N	US20090115316

TABLE 1-continued

	TABLE 1-continued	
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Anthracene- benzothiazole compounds	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq ₃ , Zrq ₄)	$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_{0} \end{bmatrix}_{3} Al$	Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7,230,107
Metal hydroxybenoquinolates	$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}_2$ Be	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)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	N-N O	Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds	N N N N N N N N N N N N N N N N N N N	Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds	$F \longrightarrow F \longrightarrow$	J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triazine complexes	$F \longrightarrow F$	US20040036077
Zn (NAN) complexes	N Zn SO ₂	U.S. Pat. No. 6,528,187

EXPERIMENTAL

Compound Examples

Example 1

Synthesis of Compound 1

[0100]

$$\underset{H}{\underbrace{\bigvee_{N}}} \underbrace{\text{KI/KIO}_{3}}$$

Synthesis of 3-iodo-9H-carbazole

[0101] To a solution of 9H-carbazole (5.57 g, 33.3 mmol) and KI (3.68 g, 22.2 mmol) in AcOH (92 mL) was heated to 100° C. for 1 h. KIO₃ (3.57 g, 16.7 mmol) was added in portions to the solution, and the resulting mixture was stirred for another 2 h at 100° C. The mixture was poured into water (500 mL) and the precipitation was collected by filtration and washed with hot water. Recrystallization was made in DCM to afford 6.8 g (70%) of product as a white solid.

Synthesis of 9-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole

[0102] To a solution of 3-bromo-9-phenyl-9H-carbazole (20.3 g, 63 mmol) in THF (150 mL) at -78° C. was added

47.25 mL (75.8 mmol) of n-butyllithium (1.6 M in hexane). The mixture was stirred at –78° C. for 1 h. 21 mL (100 mmol) of 2-isopropoxy-4,4,5,5-tetramethyl-[1,3,2]-dioxaborolane was added to the solution, and the resulting mixture was warmed to room temperature and stirred for 8 h. The mixture was poured into water and extracted with dichloromethane. The organic extracts were washed with brine and dried over magnesium sulfate. The solvent was removed by rotary evaporation, and recrystallization was made in hexane to afford 19.3 g (83%) of product as a white solid.

Synthesis of 3-(9-phenyl-9H-carbazole 3-(9-phenyl-9H-carbazole

[0103] To a solution of 3-iodo-9H-carbazole (879 mg, 3.0 mmol), $Pd(PPh_3)_4$ (165 mg, 0.15 mmol), 9-phenyl-3-(4,4,5, 5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (1.29 g, 4.5 mmol) and K_3PO_4 (1.8 g, 18.0 mmol) in dioxane (5 mL). The solution was heated to 85° C. with vigorous stirring for 48 h under argon atmosphere. The mixture was poured into water and extracted with DCM. The organic extracts were washed with brine and dried over MgSO₄. The solvent was removed by rotary evaporation, and recrystallization was made in DCM to afford 900 mg (74%) of product.

Synthesis of 9-(4,6-diphenyl-1,3,5-triazin-2-yl)-3-(9-phenyl-9H-carbazol-3-yl)-9H-carbazole (Compound 1)

[0104] To a solution of sodium hydride (100 mg, 3.0 mmol) and 3-(9-phenyl-9H-carbazol-3-yl)-9H-carbazole (816 mg, 2.0 mmol) in dry DMF (40 mL) was stirred at room temperature for 1 h under argon atmosphere. 2-Chloro-4,6-diphenyl-1,3,5-triazine (448 mg, 1.67 mmol) was added to the solution at room temperature, then refluxed overnight. The mixture was poured into water and the precipitation was collected by filtration and washed with water, methanol and DCM to get 800 mg (75%) yellow solid.

Device Examples

[0105] All device examples were fabricated by high vacuum ($<10^{-7}$ Torr) thermal evaporation. The anode electrode is 800 Å of indium tin oxide (ITO). The cathode con-

Н2

Н1

sisted 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 H₂O and O₂) immediately after fabrication, and a moisture getter was incorporated inside the package.

[0106] As used herein, the following compounds have the following structures:

-continued

НЗ

[0107] Particular devices are provided. The organic stack of the Device Examples 1 and 2 consisted of sequentially, from the ITO surface, 100 Å of E1 as the hole injection layer (HIL), 300 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl $(\alpha$ -NPD) as the hole transporting layer (HTL), 300 Å of host doped with E1 as the emissive layer (EML), 100 Å of H2 as the blocking layer (BL), and 400 Å of Alq as the electron transporting layer (ETL).

[0108] Comparative Device Examples 1 and 2 were fabricated similarly to Device Examples 1 and 2, except H3 was used as host.

[0109] Device structures for Device Examples 1 and 2 are provided in Table 2 and the corresponding measured device data is provided in Table 3.

TABLE 2

VTE PHOLEDs									
Example	BL ETL								
Example 1 Example 2 Comparative Example 1	E1 E1 E1	NPD NPD NPD	Compound 1 Compound 1 H3	E1 5% E1 10% E1 5%	H2 Alq H2 Alq H2 Alq				
Comparative Example 2	E1	NPD	Н3	E1 10%	H2 Alq				

TABLE 3

VTE device data										
						At 100	At 40 mA/cm ²			
	1931 CIE			FWHM	Voltage	LE	EQE	PE	L_0	LT80%
Example	x	у	λ_{max}	(nm)	(V)	(Cd/A)	(%)	(lm/W)	(nits)	(h)
Example 1 Example 2		0.623 0.619	520 522	66 69	5.7 5.6	40.6 47.4	11.3 13.2	22 2 26.4	12,769 15,048	86 83
Comp. Example 1		0.628	520	64	5.7	45.5	12.7	25.1	12,635	46

TABLE 3-continued

VTE device data										
	v				TE device		at 1000 nits At 40 m			
	1931 CIE		FWHM	Voltage	LE	EQE	PE	Lo	LT80%	
Example	x	у	λ_{max}	(nm)	(V)	(Cd/A)	(%)	(lm/W)	(nits)	(h)
Comp. Example 2	0.317	0.630	520	64	5.2	54.4	15.1	32.6	16,264	29

[0110] Device Examples 1 and 2 showed green PHOLEDs with Compound 1 as host with different E1 doping concentrations. The comparative examples used H3 (i.e., CBP, a commonly used PHOLED host) as the host. As can be seen from the table, devices with Compound 1 as host had comparative operating voltage, slightly lower efficiency than devices with H3 as the host. However, the device operating lifetime was much higher than comparative examples. Device Example 1 almost doubled the lifetime of Comparative Example 2 almost tripled the lifetime of Comparative Example 2 (83 h vs. 29 h). Therefore, Compound 1 is an excellent host material for phosphorescent OLEDs.

[0111] It is understood that the various embodiments described herein are 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 includes 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.

1. A compound having the formula:

$$R_3$$
 R_4
 R_4
 R_4
 R_4
 R_4

wherein R₁, R₂, R₃, and R₄ may represent mono, di, tri, or tetra substitutions;

wherein R₁, R₂, R₃, and R₄ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl;

wherein Ar₁, Ar₂, and Ar₃ are independently selected from aryl or heteroaryl; and

wherein X is C or N.

- 2. The compound of claim 1, wherein ${\rm Ar_1}, {\rm Ar_2},$ and ${\rm Ar_3}$ are further substituted.
- 3. The compound of claim 1, wherein Ar_1 , Ar_2 , and Ar_3 are independently selected from the group consisting of phenyl, pyridine, naphthalene, biphenyl, terphenyl, fluorene, dibenzofuran, dibenzothiophene, phenanthrene, and triphenylene; and
 - wherein Ar₁, Ar₂, and Ar₃ are independently further substituted with a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl, wherein the substituent is not an aryl or heteroaryl fused directly to Ar₁, Ar₂, and Ar₃.
- **4**. The compound of claim **1**, wherein Ar_1 and Ar_2 are independently selected from the group consisting of phenyl, pyridine, and naphthalene.
- 5. The compound of claim 1, wherein Ar_3 is selected from the group consisting of phenyl, biphenyl, dibenzofuran, and dibenzothiophene.
- **6**. The compound of claim **1**, wherein R_1, R_2, R_3 , and R_4 are hydrogen.
- 7. The compound of claim 1, wherein the compound is selected from the group consisting of:

-continued -continued

Compound 2

-continued -continued

Compound 6

Compound 7

Compound 10

-continued -continued

Compound 14

-continued -continued

-continued -continued

Compound 26

Compound 30

Compound 31

Compound 34

Compound 38

Compound 41

-continued -continued

Compound 46

-continued -continued

Compound 50

Compound 58

Compound 61

-continued -continued

Compound 66

-continued -continued

Compound 70

Compound 74

-continued -continued

-continued -continued

Compound 82

-continued

Compound 86

Compound 88

Compound 90

-continued -continued

Compound 94

Compound 98

Compound 110

Compound 118

Compound 122

Compound 126

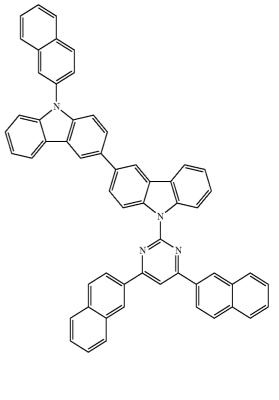
Compound 130

Compound 133

Compound 138

-continued -continued

Compound 142



-continued -continued

Compound 150

-continued -continued

Compound 154

Compound 158

-continued -continued

-continued -continued

Compound 166

Compound 174

-continued -continued

Compound 178

Compound 179

-continued

Compound 182

8. A first device comprising an organic light emitting device, further comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, wherein the organic layer comprises a compound having the formula:

Formula I

$$R_3$$
 R_4
 R_4
 R_4
 R_4

wherein R₁, R₂, R₃, and R₄ may represent mono, di, tri, or tetra substitutions;

wherein R₁, R₂, R₃, and R₄ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl;

wherein Ar₁, Ar₂, and Ar₃ are independently selected from aryl or heteroaryl; and

wherein X is C or N.

- 9. The device of claim 8, wherein ${\rm Ar_1},\,{\rm Ar_2},\,{\rm and}\,{\rm Ar_3}$ are further substituted.
- 10. The device of claim 8, wherein Ar_1 , Ar_2 , and Ar_3 are independently selected from the group consisting of phenyl, pyridine, naphthalene, biphenyl, terphenyl, fluorene, dibenzofuran, dibenzothiophene, phenanthrene, and triphenylene; and
 - wherein Ar_1 , Ar_2 , and Ar_3 are independently further substituted with a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, aryl and heteroaryl, wherein the substituent is not an aryl or heteroaryl fused directly to Ar_1 , Ar_2 , and Ar_3 .
- 11. The device of claim 8, wherein Ar_1 and Ar_2 are independently selected from the group consisting of phenyl, pyridine, and naphthalene.
- 12. The device of claim 8, wherein Ar_3 is selected from the group consisting of phenyl, biphenyl, dibenzofuran, and dibenzothiophene.
- 13. The device of claim 8, wherein R_1 , R_2 , R_3 , and R_4 are hydrogen.

14. The device of claim 8, wherein the compound is selected from the group consisting of:

-continued

Compound 13

-continued -continued

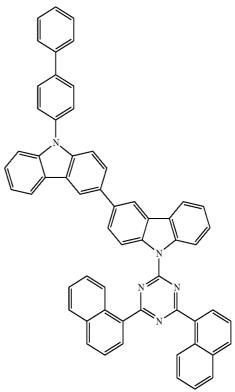
Compound 21

Compound 25

Compound 28

-continued -continued

Compound 29



Compound 33

Compound 36

Compound 40

-continued -continued

Compound 46

Compound 56

-continued -continued

Compound 53

-continued -continued

Compound 61

Compound 65

-continued -continued

-continued -continued

Compound 81

Compound 82

Compound 83

-continued -continued

-continued -continued

Compound 93

Compound 104

-continued -continued

-continued -continued

Compound 105

Compound 133

-continued -continued

Compound 141

Compound 142

Compound 145

-continued -continued

Compound 153

Compound 156

Compound 157

Compound 161

Compound 163

-continued -continued

-continued -continued

Compound 173

-continued -continued

Compound 181

Compound 182

-continued

- 15. The device of claim 8, wherein the organic layer is deposited using solution processing.
- ${\bf 16}.$ The device of claim ${\bf 8},$ wherein the organic layer is an emissive layer and the compound having Formula I is a host.
- 17. The device of claim 16, wherein the organic layer further comprises an emissive dopant having the structure:

$$\begin{bmatrix} \\ \\ \\ \\ \\ \end{bmatrix}_2$$
 D23

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

D42

D41

-continued

$$\begin{array}{c|c} & & & D46 \\ \hline \\ & & \\ & & \\ \end{array}$$

$$\begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}$$

- 18. The device of claim 8, wherein the first device is a consumer product.
- 19. The device of claim 8, wherein the first device is an organic light emitting device.

* * * * *



专利名称(译)	用于oleds的双咔唑化合物		
公开(公告)号	US20130140549A1	公开(公告)日	2013-06-06
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外部链接	Espacenet USPTO		

摘要(译)

提供了包含双咔唑核的新型有机化合物。特别地,该化合物具有在3位被三嗪或嘧啶取代的3,3'-二咔唑核。该化合物可用于有机发光器件中,以提供具有改进的效率和改善的寿命的器件。

