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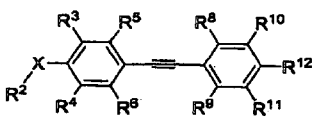

(1)

(57) Abstract: Disclosed herein are compounds represented by Formula (1). Compositions and light-emitting devices related thereto are also disclosed.

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EMISSIVE DIARYL ACETYLENES

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application claims the benefit of United States Provisional Application No. 61/184,110, filed June 4, 2009, which is incorporated by reference herein in its entirety.

BACKGROUND

Field of the Invention

[0002] This invention relates to light-emitting compounds or compositions and light-emitting devices that include the light-emitting compounds or compositions.

Description of the Related Art

[0003] Organic light-emitting devices (OLEDs) have been widely developed for flat panel displays, and are moving fast towards solid state lighting (SSL) applications. Organic Light Emitting Diodes (OLEDs) comprise a cathode, a hole transporting layer, an emissive layer, an electron transporting layer, and an anode. Light emitted from an OLED device is the result of recombination of positive charges (holes) and negative charges (electrons) inside an organic (emissive) layer. The holes and electrons combine within a single molecule or a small cluster of molecules to generate excitons, which are molecules in an excited state, or groups of organic molecules bound together in an excited state. When the organic molecules release the required energy and return to its stable state, photons are generated. The organic compound or group of compounds which emit the photons is referred as an electro-fluorescent material or electro-phosphorescent material depending on the nature of the radiative process. Thus the OLED emissive compounds may be selected for their ability to absorb primary radiation and emit radiation of a desired wavelength. For blue emitters, for example, emission within principle emission bands of 440 to 490 nm is desirable.

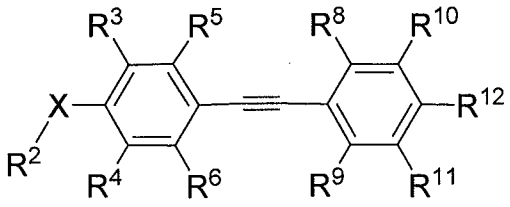
[0004] SSL applications may require white OLED device to achieve greater than 1,500 lm brightness, a color rendering index (CRI) greater than 70, and an operating time greater than 100,000 hours at 1,000 lm/w. There are many approaches for generating white light from an OLED, but two common approaches are: direct combination of red, blue, and green light using either lateral patterning or vertical stacking of three emitters; and partial down conversion of blue light in combination with yellow phosphors. Both of these common approaches may be more effective if a highly efficient chemical- and

photo-stable blue dye is employed. However, blue emitters may be less stable than dyes which emit other colors. Furthermore, and there are very few blue emitting devices showing CIE y value below 0.2 yet still with respectable efficiency. Thus, the development of deep blue emitters with good stability and high luminescence efficiency is desirable to effectively reduce power consumption and generating emission of different colors.

[0005] Diphenyl acetylene compounds have been used as additives in organic photoreflective polymer composites for electrooptic, photorefractive and liquid crystal applications (see for example, US 2006/0050354 and US 2006/000363). Thompson, et al (US Patent No. 6,210,814) described a polarization dopant molecule that contributed to the local dipole moment to spectrally shift the emission of a separate emissive dopant. Thompson, et al (US Patent No. 6,045,930) describes a [tris-diphenylacetylene amine] compound However, none of these compounds were described as blue emitting fluorescent compounds. Thus, the development of deep blue emitters with good stability and high luminescence efficiency is desirable to effectively reduce power consumption and generating emission of different colors.

SUMMARY OF THE INVENTION

[0006] One embodiment provides compounds that are useful as deep blue emitters. These compounds are represented by a formula:



(Formula 1);

wherein R^2 is C_{1-30} alkyl, or $C_{1-30}O_{1-15}$ ether; R^3, R^4, R^5, and R^6 are independently selected from –H, –F, –Cl, –Br, –I, C_{1-10} alkyl, $C_{1-10}O$ ether, and optionally substituted C_{6-10} aryl; X is –O- or $-NR^7-$, wherein R^7 is –H, C_{1-12} alkyl, or $C_{1-12}O_{1-6}$ ether; R^8 and R^9 are independently —H, –F, –Cl, –Br, –I, C_{1-10} alkyl or C_{1-10} ether; and R^{10}, R^{11} and R^{12} are independently halogen, –CN, or $-NO_2$.

[0007] Another embodiment is a light-emitting device, comprising an anode layer; a cathode layer; and a light-emitting layer positioned between the anode layer and the cathode layer, the light-emitting layer comprising a compound disclosed herein.

BRIEF DESCRIPTION OF THE DRAWINGS

[0008] Figure 1 shows an exemplary configuration of an organic light-emitting device incorporating an embodiment of deep blue emissive compound of Formula 1.

[0009] Figure 2 is a graph depicting the emissive spectrum and CIE coordinates of an embodiment of anorganic light-emitting device of Fig. 1.

[0010] Figure 3 is a graph depicting the current density and luminance of an embodiment of a device of Figure 1 as a function of the driving voltage.

[0011] Figure 4 is a graph depicting the External Quantum Efficiency (EQE) and luminous efficiency of an embodiment of a device of Figure 1, as a function of current density.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

[0012] Reference to a compound also includes any salts of that compound.

[0013] Unless otherwise indicated, when a structural feature such as alkyl or aryl is referred to as being "optionally substituted," it is meant that the feature may have no substituents or may have one or more substituents. A feature that is "substituted" has one or more substituents. In some embodiments, each substituent is composed of 0-20 carbon atoms, 0-47 hydrogen atoms, 0-5 oxygen atoms, 0-2 sulfur atoms, 0-3 nitrogen atoms, 0-1 silicon atoms, 0-7 fluorine atoms, 0-3 chlorine atoms, 0-3 bromine atoms, and 0-3 iodine atoms. Examples include, but are not limited to, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, cycloalkynyl, aryl, heteroaryl, heteroalicyclyl, aralkyl, heteroaralkyl, (heteroalicyclyl)alkyl, hydroxy, protected hydroxyl, alkoxy, aryloxy, acyl, ester, mercapto, alkylthio, arylthio, cyano, halogen, carbonyl, thiocarbonyl, O-carbamyl, N-carbamyl, O-thiocarbamyl, N-thiocarbamyl, C-amido, N-amido, S-sulfonamido, N-sulfonamido, C-carboxy, protected C-carboxy, O-carboxy, isocyanato, thiocyanato, isothiocyanato, nitro, silyl, sulfenyl, sulfinyl, sulfonyl, haloalkyl, haloalkoxy, trihalomethanesulfonyl, trihalomethanesulfonamido, and amino, including mono- and di-substituted amino groups, and the protected derivatives thereof.

[0014] As used herein, the term "aryl" refers to an aromatic ring or ring system. Exemplary aryl groups are phenyl, naphthyl, etc.

[0015] As used herein, the term "C_{6-10} aryl" refers to aryl where the ring or ring system has from 6-10 carbon atoms. "C_{6-10} aryl" does not characterize or limit any hydrogen or substituents attached to the ring atoms.

[0016] As used herein, the term "heteroaryl" refers to an aromatic ring or ring system having one or more atoms selected from nitrogen, oxygen, or sulfur in an aromatic ring. Examples include pyridinyl, pyridazinyl, triazinyl, pyridinyl, pyrimidinyl, pyrazinyl, benzoimidazolyl, indolyl, benzooxazolyl, etc.

[0017] As used herein, the term "$C_{3-10}O_{0-1}N_{1-3}$ heteroaryl" refers to heteroaryl where the atoms of the ring or ring system has from 3-10 carbon atoms, from 0-1 oxygen atoms, and from 1-3 nitrogen atoms. "$C_{3-10}O_{0-1}N_{1-3}$ heteroaryl" does not characterize or limit any hydrogen or substituents attached to the ring atoms.

[0018] As used herein, the term "alkyl" refers to a moiety consisting of carbon and hydrogen containing no double or triple bonds. Alkyl may be linear, branched, cyclic, or a combination thereof, and contain from one to thirty-five carbon atoms. Examples of alkyl groups include but are not limited to methyl, ethyl, propyl, isopropyl, cyclopropyl, n-butyl, iso-butyl, tert-butyl, cyclobutyl, pentyl isomers, cyclopentane, hexyl isomer, cyclohexane, and the like.

[0019] As used herein, the term "linear alkyl" refers to $-(CH_2)_qCH_3$, where q is 0-34.

[0020] As used herein, the term "C_{1-30} alkyl" refers to alkyl having from 1 to 30 carbon atoms such as methyl, ethyl, propyl isomers, butyl isomers, cyclobutyl isomers, pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomer, heptyl isomers, cycloheptyl isomers, octyl isomers, cyclooctyl isomers, nonyl isomers, cyclononyl isomers, decyl isomer, cyclodecyl isomers, etc., up to 30 carbon atoms.

[0021] As used herein, the term "C_{1-12} alkyl" refers to alkyl having from 1 to 12 carbon atoms such as methyl, ethyl, propyl isomers, butyl isomers, cyclobutyl isomers, pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomer, heptyl isomers, cycloheptyl isomers, octyl isomers, cyclooctyl isomers, nonyl isomers, cyclononyl isomers, decyl isomer, cyclodecyl isomers, etc., up to 12 carbon atoms.

[0022] As used herein, the term "C_{1-10} alkyl" refers to alkyl having from 1 to 10 carbon atoms such as methyl, ethyl, propyl isomers, butyl isomers, cyclobutyl isomers, pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomer, heptyl isomers, cycloheptyl isomers, octyl isomers, cyclooctyl isomers, nonyl isomers, cyclononyl isomers, decyl isomer, cyclodecyl isomers, etc.

[0023] As used herein, the term "ether" refers to a moiety consisting of carbon, hydrogen, and single bonded oxygen, i.e. –O-, provided that –O-O- is not present.

Examples include: –O-alkyl, such as –O-methyl, -O-ethyl, -O-propyl, -O-isopropyl, etc.; -alkyl-O-alkyl, such as –methyl-O-methyl, -methyl-O-ethyl, -methyl-O-isopropyl, etc.; and $-(CH_2CH_2O)_n-$.

[0024] As used herein, the term "$C_{1-30}O_{1-15}$ ether" refers to ether having from 1-30 carbon atoms, from 1-15 oxygen atoms, and hydrogen. Examples include, but are not limited to, $-(CH_2CH_2O)_nCH_3-$ where n is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, or 14; $-[CH(CH_3)CH_2O]_nCH_3-$ where n is 1, 2, 3, 4, 5, 6, 7, 8, or 9; and $-(CH_2)_o-O-(CH_2)_pCH_3$ where o + p is from 1-29.

[0025] As used herein, the term "$C_{1-10}O$ ether" refers to ether having from 1-10 carbon atoms, 1 oxygen atom, and hydrogen, such as: $-O-C_xH_{2x+1}$ or $-OC_xH_{2x}$, where x is 1-10, e.g. –O-methyl, -O-ethyl, $-O-C_3H_7$, $-OC_3H_6$, $-OC_4H_9$, $-OC_5H_{11}$, $-O-C_5H_{10}$, etc.

[0026] As used herein, the term "work function" of a metal refers to a measure of the minimum energy required to extract an electron from the surface of the metal.

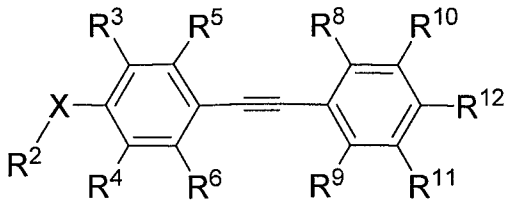
[0027] As used herein, the term "high work function metal" refers to a metal or alloy that easily injects holes and typically has a work function greater than or equal to 4.5.

[0028] As used herein, the term "low work function metal" refers to a metal or alloy that easily loses electrons and typically has a work function less than 4.3.

[0029] A material is white light-emitting if it emits white light. White light is light having the approximate CIE color coordinates (X =1/3, Y = 1/3). The CIE color coordinates (X=1/3, Y=1/3) is defined as the achromatic point. The X and Y color coordinates are weights applied to the CIE primaries to match a color. A more detailed description of these terms may be found in CIE 1971, International Commission on Illumination, Colorimetry: Official Recommendations of the International Commission on Illumination, Publication CIE No. 15 (E-1.3.1) 1971, Bureau Central de la CIE, Paris, 1971 and in F. W. Billmeyer, Jr., M. Saltzman, Principles of Color Technology, 2nd edition, John Wiley & Sons, Inc., New York, 1981, both of which are hereby incorporated by reference in their entireties. The color rendering index (CRI) refers to the ability to render various colors and has values ranging from 0 to 100, with 100 being the best.

[0030] A material is "deep blue" emitting if it emits deep blue light. Deep Blue light is light having the approximate CIE color coordinates $X \leq 0.2$ and $Y \leq 0.1$). Non-limiting examples include X= [0.14], Y = [0.08], or X = 0.16 and Y = 0.10 (CIE 1931).

[0031] Some embodiments provide compounds that are useful as deep blue emitters. The compounds are represented by a formula 1:



(Formula 1);

wherein R^2 is C_{1-30} alkyl, or $C_{1-30}O_{1-15}$ ether; R^3, R^4, R^5, and R^6 are independently selected from –H, –F, –Cl, –Br, –I, C_{1-10} alkyl, $C_{1-10}O$ ether, and optionally substituted C_{6-10} aryl; X is –O- or $-NR^7-$, wherein R^7 is –H, C_{1-12} alkyl, or $C_{1-12}O_{1-6}$ ether; R^8 and R^9 are independently —H, –F, –Cl, –Br, –I, C_{1-10} alkyl or C_{1-10} ether; and R^{10}, R^{11} and R^{12} are independently halogen, –CN, or $-NO_2$.

[0032] In some embodiments, if R^2 is methyl, ethyl, propyl, or isopropyl, at least one of R^3, R^4, R^5, and R^6 is not –H. In some embodiments, if R^2 is linear alkyl, at least one of R^3, R^4, R^5, and R^6 is not –H.

[0033] Some embodiments comprise blue emitting compounds characterized by substituted diphenyl acetylene compounds comprising electron donating substituents on one phenyl ring and electron withdrawing substituents on the other phenyl ring. Electron withdrawing groups and electron donating groups have the ordinary meaning used by one skilled in the art. In some embodiments, an electron withdrawing group is a moiety which is more electronegative than hydrogen, or alternatively, withdraws more electron density from the phenyl ring than hydrogen does. In some embodiments, an electron donating group is a moiety which is less electronegative than hydrogen, or alternatively, donates more electron density into the phenyl ring than hydrogen does.

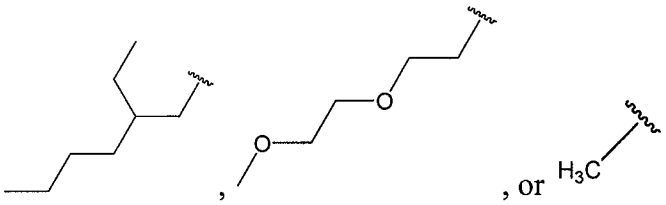
[0034] While this invention is not limited by any particular theory or mechanism, it is believed that in some embodiments, a blue emitting compound may have a "push" (electron donating) end and a "pull" (electron-withdrawing or electron-accepting) end which affects the orbital structure of an emissive molecule to the extent that the energy levels of the molecule may shift from an ultraviolet emitting compound to a deep blue emitting compound. Thus in some embodiments, X of Formula 1, at the "push" end of the blue emitting compound, comprises an electron donating hetero-atom, N, O or S, or in a preferred embodiment an O or an N, or in a still more preferred embodiment an O at the "push" end. In another embodiment, the phenyl group proximal to the "push" end comprises electron donating groups for at least one, or alternatively all,

of R^3, R^4, and R^4. In some embodiments, the electron donating group may be a methyl group, an isopropyl group, a phenyloxy group, a benzyloxy group, a dimethylamino group, a diphenylamino group, a pyrrolidine group, or a phenyl group. In some embodiments, at least one, or alternatively all, of R^{10}, R^{11} and R^{12} at the "pull" end of the deep blue emitting compound, can independently be an electron withdrawing group, such as a fluoro group, a cyano group, a trifluoromethyl group, or a phenyl group with a trifluoromethyl moiety

[0035] In some embodiments, R^2 may also be, but is not limited to, C_{1-12} alkyl or C_{4-30} alkyl. "C_{4-30} alkyl" is alkyl having from 4 to 30 carbon atoms such as butyl isomers, cyclobutyl isomers, pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomer, heptyl isomers, cycloheptyl isomers, octyl isomers, cyclooctyl isomers, nonyl isomers, cyclononyl isomers, decyl isomer, cyclodecyl isomers, etc., up to 30 carbon atoms.

[0036] In some embodiments, R^2 may also be, but is not limited to, $C_{1-9}O_{1-4}$ ether. "$C_{1-9}O_{1-4}$ ether" is ether having from 1-9 carbon atoms, 1-4 oxygen atoms, and hydrogen. Examples include, but are not limited to, $-CH_2CH_2OCH_3$, $-CH_2CH_2OCH_2CH_2OCH_3$, $-CH_2CH(CH_3)OCH_3$, $-CH_2CH(CH_3)OCH_2CH(CH_3)OCH_3$, $-CH_2CH_2OCH_2CH_2OCH_3$, $-CH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$, etc.

[0037] In some embodiments, R^2 is selected from the following group:



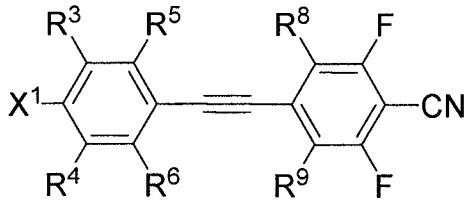
, , or .

[0038] In some embodiments, if R^2 is methyl, ethyl, propyl, or isopropyl, at least one of R^3, R^4, R^5, and R^6 is not –H. In other words, if R^2 is methyl, ethyl, propyl, or isopropyl, then (1) R^3 is -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl; and R^4, R^5, and R^6 are independently –H, -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl; (2) R^4 is -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl; and R^3, R^5, and R^6 are independently –H, -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl; (3) R^5 is -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl; and R^3, R^4, and R^6 are independently –H, -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, and optionally substituted C_{6-10} aryl; or (4) R^6 is -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, and optionally substituted C_{6-10}

$_{10}$ aryl; and R^3, R^4, and R^5 are independently –H, -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl.

[0039] In some embodiments, R^3, R^4, R^5, and R^6 are independently selected from: -H, $–CH_3$, isopropyl, and $-OCH_3$. In some embodiments R^5 is -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl. In some embodiments R^5 and R^6 are independently -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, or optionally substituted C_{6-10} aryl. In some embodiments, R^5 is -F, -Cl, -Br, -I, C_{1-4} alkyl, or $C_{1-4}O$ ether. In some embodiments, R^5 and R^6 are independently -F, -Cl, -Br, -I, C_{1-4} alkyl, or $C_{1-4}O$ ether. In some embodiments, R^5 is $–CH_3$, isopropyl, or $-OCH_3$.

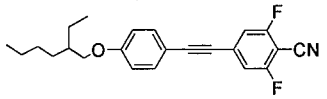
[0040] In some embodiments, the deep blue emissive compound may be represented by the following formula:

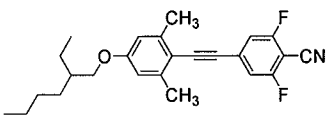


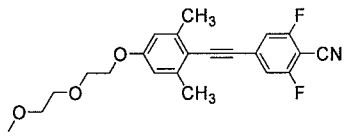
(Formula 2)

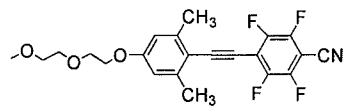
wherein X^1 is $–O(CH_2CH_2O)_n-C_oH_{2o+1}$; n is 0, 1, 2, 3, or 4; o is 1, 2, 3, 4, 5, 6, 7, or 8; R^3, R^4, R^5, and R^6 are independently –H , C_{1-4} alkyl, or C_{1-4} O-alkyl; and R^8 and R^9 are independently –H, –F, -Cl, -Br, or –I. In these embodiments, both the o subscript for C and the o which is part of the subscript for H are the same value.

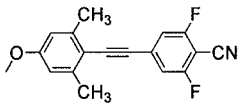
[0041] Non-limiting examples of a compound of Formula 1 include:

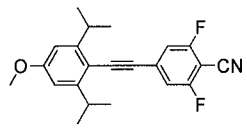


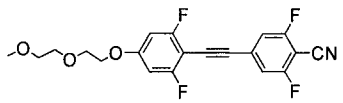


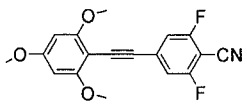












[0042] Another embodiment described herein relates to a light emitting device that can include: an anode layer comprising a high work function metal; a cathode layer

comprising a low work function metal; and a light-emitting layer positioned between, and electrically connected to, the anode layer and the cathode layer.

[0043] The compounds or compositions described herein can be incorporated into light-emitting devices in various ways. For example, an embodiment provides a light-emitting device, comprising: an anode layer comprising a high work function metal; a cathode layer comprising a low work function metal; and a light-emitting layer positioned between, and electrically connected to, the anode layer and the cathode layer. The light-emitting layer comprises the compounds or compositions disclosed herein.

[0044] An anode layer may comprise a conventional material such as a metal, mixed metal, alloy, metal oxide or mixed-metal oxide, or a conductive polymer. Examples of suitable metals include the Group 1 metals, the metals in Groups 4, 5, 6, and the Group 8-10 transition metals. If the anode layer is to be light-transmitting, mixed-metal oxides of Group 12, 13, and 14 metals or alloys thereof, such as Au, Pt, and indium-tin-oxide (ITO), may be used. The anode layer may include an organic material such as polyaniline, e.g., as described in "Flexible light-emitting diodes made from soluble conducting polymer," Nature, vol. 357, pp. 477-479 (11 June 1992). Examples of suitable high work function metals include but are not limited to Au, Pt, indium-tin-oxide (ITO), or alloys thereof. In an embodiment, the anode layer can have a thickness in the range of about 1 nm to about 1000 nm.

[0045] A cathode layer may include a material having a lower work function than the anode layer. Examples of suitable materials for the cathode layer include those selected from alkali metals of Group 1, Group 2 metals, Group 12 metals including rare earth elements, lanthanides and actinides, materials such as aluminum, indium, calcium, barium, samarium and magnesium, and combinations thereof. Li-containing organometallic compounds, LiF, and Li_2O may also be deposited between the organic layer and the cathode layer to lower the operating voltage. Suitable low work function metals include but are not limited to Al, Ag, Mg, Ca, Cu, Mg/Ag, LiF/Al, CsF, CsF/Al or alloys thereof. In an embodiment, the cathode layer can have a thickness in the range of about 1 nm to about 1000 nm.

[0046] The amount of the compounds disclosed herein in the light-emitting composition can vary. In one embodiment, the amount of a compound disclosed herein in the light-emitting layer is from about 1% to about 100% by weight of the light-emitting layer. In another embodiment, the amount of a compound disclosed herein in the light-

emitting layer is from about 1% to about 10% by weight of the light-emitting layer. In another embodiment, the amount of a compound disclosed herein in the light-emitting layer is about 3% by weight of the light-emitting layer.

[0047] The thickness of the light-emitting layer may vary. In one embodiment, the light-emitting layer has a thickness from about 20 nm to about 200 nm. In another embodiment, the light-emitting layer has a thickness in the range of about 20 nm to about 150 nm.

[0048] In another embodiment, the light-emitting layer may also be configured to emit blue light.

[0049] In some embodiments, the light-emitting layer can further include a host material. Exemplary host materials are known to those skilled in the art. For example, the host material included in the light-emitting layer can be an optionally substituted compound selected from: an aromatic-substituted amine, an aromatic-substituted phosphine, a thiophene, an oxadiazole, 2-(4-biphenylyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (PBD), 1,3-bis(N,N-t-butyl-phenyl)-1,3,,4-oxadiazole (OXD-7), a triazole, 3-phenyl-4-(1'-naphthyl)-5-phenyl-1,2,4-triazole (TAZ), 3,4,5-Triphenyl-1,2,3-triazole, 3,5-Bis(4-tert-butyl-phenyl)-4-phenyl[1,2,4]triazole, an aromatic phenanthroline, 2,9-dimethyl-4,7-diphenyl-phenanthroline (bathocuproine or BCP), 2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline, a benzoxazole, a benzothiazole, a quinoline, aluminum tris(8-hydroxyquinolate) (Alq3), a pyridine, a dicyanoimidazole, cyano-substituted aromatic, 1,3,5-tris(2-N-phenylbenzimidazolyl)benzene (TPBI), 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α-NPD), N,N'-bis(3-methylphenyl)N,N'-diphenyl-[1,1'-biphenyl]-4,4'-diamine (TPD), 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (M14), 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (HMTPD), 1,1-Bis(4-bis(4-methylphenyl) aminophenyl) cyclohexane, a carbazole, 4,4'-N,N'-dicarbazole-biphenyl (CBP), poly(9-vinylcarbazole) (PVK), N,N'N"-1,3,5-tricarbazoloylbenzene (tCP), a polythiophene, a benzidine, N,N'-bis(4-butylphenyl)-N,N'-bis(phenyl)benzidine, a triphenylamine, 4,4',4"-Tris(N-(naphthylen-2-yl)-N-phenylamino)triphenylamine, 4,4',4''-tris(3-methylphenylphenylamino)triphenylamine (MTDATA), a phenylenediamine, a polyacetylene, and a phthalocyanine metal complex.

[0050] It is understood to those skilled in the art that the groups described above as possible hosts can function as hole-transport materials or electron-transport

materials. In one embodiment, the light-emitting layer further comprises a hole-transport material or an electron-transport material.

[0051] Exemplary hole-transport materials include 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α-NPD), N,N'-bis(3-methylphenyl)N,N'-diphenyl-[1,1'-biphenyl]-4,4'-diamine (TPD), 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (M14), 4,4',4'-tris(3-methylphenylphenylamino)triphenylamine (MTDATA), 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (HMTPD), N,N'N"-1,3,5-tricarbazoloylbenzene (tCP), 4,4'-N,N'-dicarbazole-biphenyl (CBP), poly(9-vinylcarbazole) (PVK), 3,4,5-Triphenyl-1,2,3-triazole, 3,5-Bis(4-tert-butyl-phenyl)-4-phenyl[1,2,4]triazole, 2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline, 1,1-Bis(4-bis(4-methylphenyl) aminophenyl) cyclohexane, N,N'-bis(4-butylphenyl)-N,N'-bis(phenyl)benzidine, 4,4',4"-Tris(N-(naphthylen-2-yl)-N-phenylamino)triphenylamine, and copper phthalocyanine.

[0052] The amount of the hole transport material in the light-emitting layer is from about 1% to about 99% by weight, or alternatively, from about 30% to about 70% by weight, of the light-emitting layer.

[0053] If desired, additional layers may be included in the light-emitting device. Additional layers that may be included include an electron injection layer (EIL), electron transport layer (ETL), hole blocking layer (HBL), exciton blocking layer (EBL), hole transport layer (HTL), and/or hole injection layer (HIL). In addition to separate layers, some of these materials may be combined into a single layer. For example, a hole transport material and/or an electron transport material could be incorporated into the emissive layer.

[0054] In some embodiments, the light-emitting device can include an electron injection layer e.g., between the cathode layer and the light emitting layer. In some embodiments, the lowest un-occupied molecular orbital (LUMO) energy level of the material(s) that can be included in the electron injection layer is high enough to prevent it from receiving an electron from the light emitting layer. In other embodiments, the energy difference between the LUMO of the material(s) that can be included in the electron injection layer and the work function of the cathode layer is small enough to allow efficient electron injection from the cathode. A number of suitable electron injection materials are known to those skilled in the art. Examples of suitable material(s) that can be included in the electron injection layer include but are not limited to, an

optionally substituted compound selected from the following: aluminum quinolate (Alq_3), 2-(4-biphenylyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (PBD), phenanthroline, quinoxaline, 1,3,5-tris[N-phenylbenzimidazol-z-yl] benzene (TPBI) a triazine, a metal chelate of 8-hydroxyquinoline such as tris(8-hydroxyquinoliate) aluminum, and a metal thioxinoid compound such as bis(8-quinolinethiolato) zinc. In one embodiment, the electron injection layer is aluminum quinolate (Alq_3), 2-(4-biphenylyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (PBD), phenanthroline, quinoxaline, 1,3,5-tris[N-phenylbenzimidazol-z-yl] benzene (TPBI), or a derivative or a combination thereof.

[0055] Some embodiments described herein can include an electron transport layer positioned between the cathode and light-emitting layer. Suitable electron transport materials are known to those skilled in the art. Exemplary electron transport materials that can be included in the electron transport layer are an optionally substituted compound selected from: aluminum tris(8-hydroxyquinolate) (Alq3), 2-(4-biphenylyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (PBD), 1,3-bis(N,N-t-butyl-phenyl)-1,3,,4-oxadiazole (OXD-7), 3-phenyl-4-(1'-naphthyl)-5-phenyl-1,2,4-triazole (TAZ), 2,9-dimethyl-4,7-diphenyl-phenanthroline (bathocuproine or BCP), and 1,3,5-tris[2-N-phenylbenzimidazol-z-yl]benzene (TPBI). In one embodiment, the electron transport layer is aluminum quinolate (Alq_3), 2-(4-biphenylyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (PBD), phenanthroline, quinoxaline, 1,3,5-tris[N-phenylbenzimidazol-z-yl] benzene (TPBI), or a derivative or a combination thereof.

[0056] In some embodiments, the hole transport material is incorporated into the light-emitting layer. The amount of the electron transport material in the light-emitting layer may be from about 1% to about 99% by weight, or alternatively, from about 30% to about 70% by weight, of the light-emitting layer

[0057] In some embodiments, the device can include a hole blocking layer, e.g., between the cathode and the light-emitting layer. Various suitable hole blocking materials that can be included in the hole blocking layer are known to those skilled in the art. Suitable hole blocking material(s) include but are not limited to, an optionally substituted compound selected from the following: bathocuproine (BCP), 3,4,5-triphenyl-1,2,4-triazole, 3,5-bis(4-tert-butyl-phenyl)-4-phenyl-[1,2,4] triazole, 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline, and 1,1-bis(4-bis(4-methylphenyl)aminophenyl)-cyclohexane.

[0058] In some embodiments, the light-emitting device can include an exciton blocking layer, e.g., between the light-emitting layer and the anode. In one embodiment, the band gap of the material(s) that comprise exciton blocking layer is large enough to substantially prevent the diffusion of excitons. A number of suitable exciton blocking materials that can be included in the exciton blocking layer are known to those skilled in the art. Examples of material(s) that can compose an exciton blocking layer include an optionally substituted compound selected from the following: aluminum quinolate (Alq_3), 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α-NPD), 4,4'-N,N'-dicarbazole-biphenyl (CBP), and bathocuproine (BCP), and any other material(s) that have a large enough band gap to substantially prevent the diffusion of excitons.

[0059] In some embodiments, the light-emitting device can include a hole transport layer, e.g., between the light-emitting layer and the anode. Suitable hole transport materials that can be included in the hole transport layer are known those skilled in the art. For example, hole transport material(s) that can be included in the hole transport layer are 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α-NPD), N,N'-bis(3-methylphenyl)N,N'-diphenyl-[1,1'-biphenyl]-4,4'-diamine (TPD), 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (M14), 4,4',4'-tris(3-methylphenylphenylamino)triphenylamine (MTDATA), 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (HMTPD), N,N'N"-1,3,5-tricarbazoloylbenzene (tCP), 4,4'-N,N'-dicarbazole-biphenyl (CBP), poly(9-vinylcarbazole) (PVK), 3,4,5-Triphenyl-1,2,3-triazole, 3,5-Bis(4-tert-butyl-phenyl)-4-phenyl[1,2,4]triazole, 2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline, 1,1-Bis(4-bis(4-methylphenyl) aminophenyl) cyclohexane, a carbazole, a polythiophene, a benzidine, N,N'-bis(4-butylphenyl)-N,N'-bis(phenyl)benzidine, a triphenylamine, a phenylenediamine, 4,4',4"-Tris(N-(naphthylen-2-yl)-N-phenylamino)triphenylamine, an oxadiazole, a polyacetylene and a phthalocyanine metal complex.

[0060] In some embodiments, the light-emitting device can include a hole injection layer, e.g., between the light-emitting layer and the anode. Various suitable hole injection materials that can be included in the hole injection layer are known to those skilled in the art. Exemplary hole injection material(s) include an optionally substituted compound selected from the following: a polythiophene derivative such as poly(3,4-ethylenedioxythiophene (PEDOT)/polystyrene sulphonic acid (PSS), a benzidine derivative such as N, N, N', N'-tetraphenylbenzidine, poly(N,N'-bis(4-butylphenyl)-N,N'-

bis(phenyl)benzidine), a triphenylamine or phenylenediamine derivative such as N,N'-bis(4-methylphenyl)-N,N'-bis(phenyl)-1,4-phenylenediamine, 4,4',4''-tris(N-(naphthylen-2-yl)-N-phenylamino)triphenylamine, an oxadiazole derivative such as 1,3-bis(5-(4-diphenylamino)phenyl-1,3,4-oxadiazol-2-yl)benzene, a polyacetylene derivative such as poly(1,2-bis-benzylthio-acetylene), or a phthalocyanine metal complex derivative such as phthalocyanine copper. Hole-injection materials, while still being able to transport holes, may have a hole mobility substantially less than the hole mobility of conventional hole transport materials.

[0061] Those skilled in the art recognize that the various materials described above can be incorporated in several different layers depending on the configuration of the device. In one embodiment, the materials used in each layer are selected to result in the recombination of the holes and electrons in the light-emitting layer. An example of a device configuration that incorporates the various layers described herein is illustrated schematically in Figure 1. The electron injection layer (EIL), electron transport layer (ETL), hole blocking layer (HBL), exciton blocking layer (EBL), hole transport layer (HTL), and hole injection layer (HIL) can be added to the light-emitting device using methods known to those skilled in the art (e.g., vapor deposition).

[0062] Light-emitting devices comprising the compounds or compositions disclosed herein can be fabricated using techniques known in the art, as informed by the guidance provided herein. For example, a glass substrate can be coated with a high work functioning metal such as ITO which can act as an anode. After patterning the anode layer, a light-emitting composition layer that includes a compound or a composition disclosed herein can be deposited on the anode. The cathode layer, comprising a low work functioning metal (e.g., Mg:Ag), can then be vapor evaporated onto the light-emitting composition layer. If desired, the device can also include an electron transport/injection layer, a hole blocking layer, a hole injection layer, an exciton blocking layer and/or a second light-emitting layer that can be added to the device using techniques known in the art, as informed by the guidance provided herein.

[0063] The light emitting devices described herein can be configured to emit various colors of light. For example, blue emitting compounds disclosed herein and orange emitting compound(s) can be placed in the light-emitting layer to produce white light.

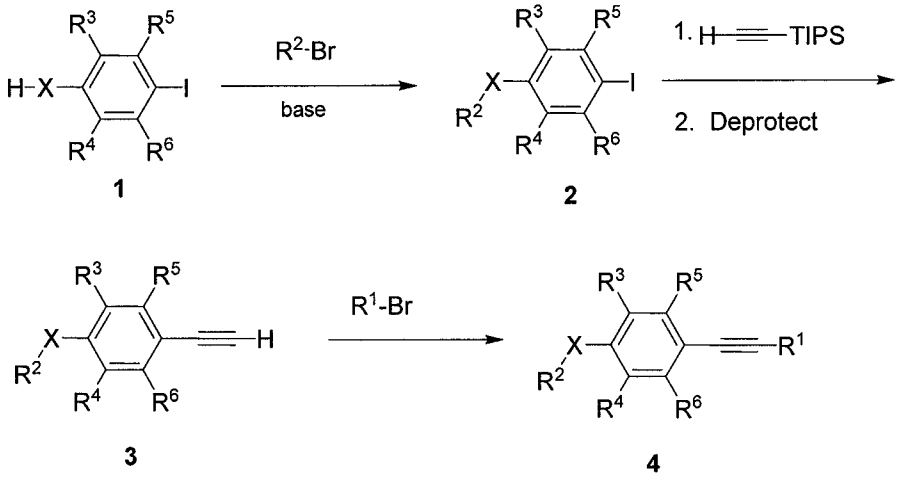
[0064] Light-emitting devices comprising blue emitter compounds can be fabricated using techniques known in the art, as informed by the guidance provided herein. For example, a glass substrate can be coated with a high work functioning metal such as Indium Tin Oxide (ITO) which can act as an anode. After patterning the anode layer, a light-emitting composition layer that includes the blue emitting compound can be deposited on the anode. The cathode layer, comprising a low work functioning metal (e.g., Mg:Ag), can then be vapor evaporated onto the light-emitting composition layer. If desired, the device can also include an electron transport/injection layer, a hole blocking layer, a hole injection layer, an exciton blocking layer and/or a second light-emitting layer that can be added to the device using techniques known in the art.

EXAMPLES

Example 1: General Synthetic Methods

[0065] While there are many ways readily apparent to those skilled in the art to prepare the compounds disclosed, general Scheme 1 illustrates a method that can be used to prepare a variety of compounds.

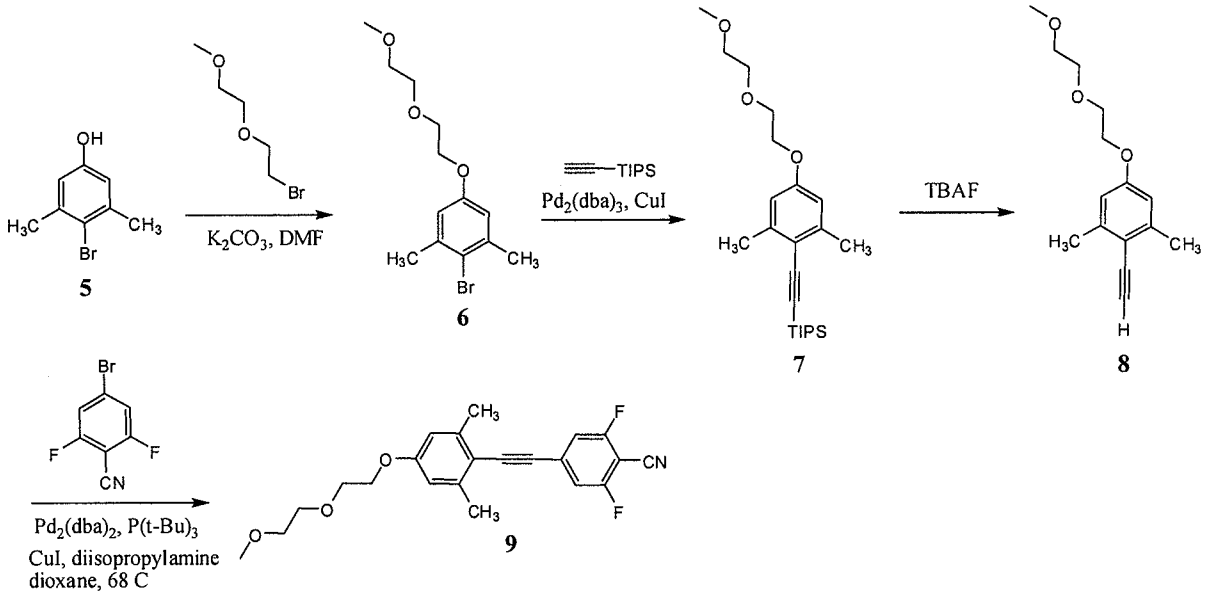
Scheme 1



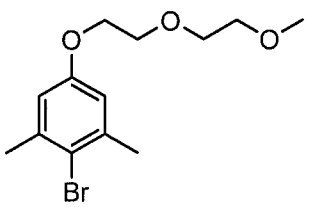
[0066] In this method, a phenyl substituted phenyl ring (compound **1**) having an amine or hydroxyl moiety (-X-H) para to a halogen such as –I, is coupled to R^2 using a catalyst such as a base (e.g. K_2CO_3) to form compound **2**. Compound **2** is then coupled to a protected acetylene, via a halogen-metal coupling reaction. The acetylene is then deprotected to yield compound **3**. The deprotected acetylene is then coupled to the second aromatic ring (i.e. R1) via a second halogen-metal coupling to form compound **4**. A variety of substitution is available the aryl rings via precursor compounds which are

readily purchased or prepared using standard reactions. Finally, a variety of R^1-Br are available via commercially available compounds and standard chemistry.

Scheme 2

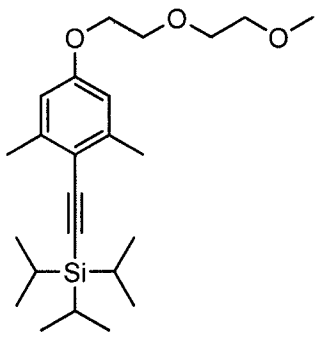


Example 1



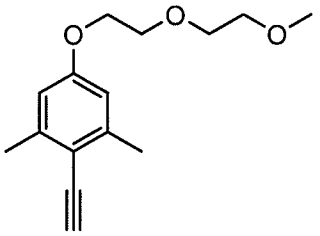
6

[0067] 4-Bromo-3, 5-dimethylphenol (10.05g, 50.0mmol) and K_2CO_3 (9.0g, 65.2mmol) was stirred for 10 minutes in DMF (25mL). 2-Bromo-(2-methoxyethoxy)-ethane was added, and the reaction mixture was heated at 45°C overnight under argon. After cooling to room temperature, the reaction mixture was poured into ~300mL DCM; filtered off white solids. Flash column (silica; 100% hexane) gave 12.95g (85% yield) of product **6**.



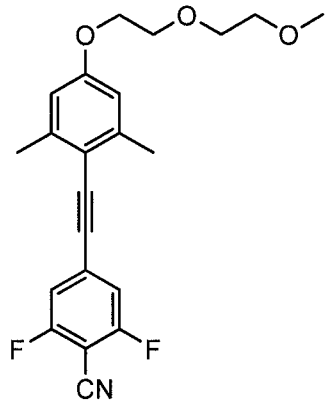
7

[0068] $Pd_2(dba)_3$ (600mg) and CuI (600mg) were added to 1,4-dioxane (75mL), and the mixture was degassed for 20 minutes. $P(t\text{-}Bu)_3$ (24mL; solution as 10% in hexanes) was added, and degassing continued for 10 minutes. 4-Bromo-3, 5-dimethyl-1-(2-(2-methoxyethoxy)ethoxy)benzene (**6**) (12.95g, 42.7mmol) and triisopropylsilylacetylene (31.09g, 171mmol) were added; and degassing was continued for 15 minutes. Diisopropylamine (18mL) was added, and reaction mixture was further degassed for 20 minutes. The mixture was heated at 90°C for 36 hours under argon. The mixture was removed from heat, cooled, poured into ~200mL of diethyl ether, and grey solids formed were filtered off. The filtrate was purified by flash column (silica; 100% hexane to 10% ethyl acetate in hexane gradient) to give 13.20g of product **7** (76% yield).



8

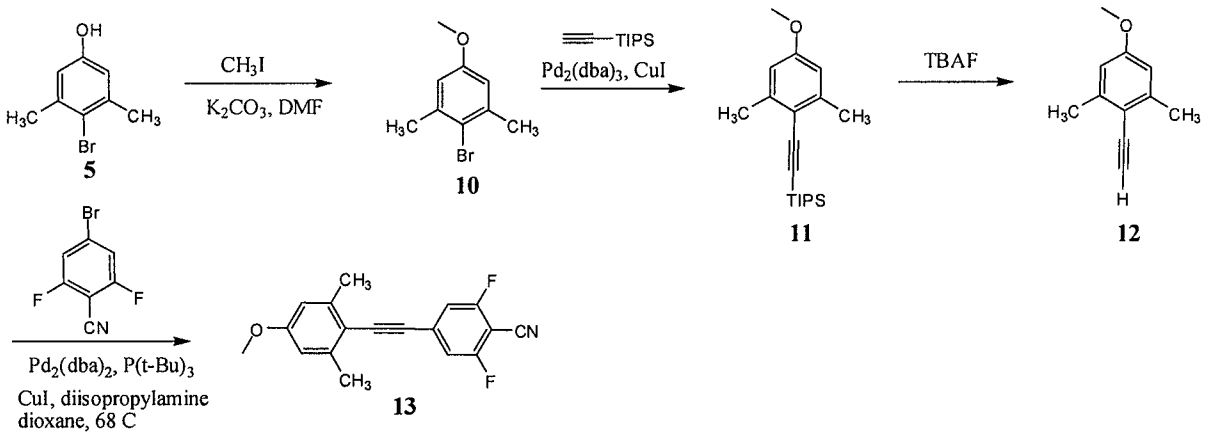
[0069] 3, 5-dimethyl-1-(2-(2-methoxyethoxy)ethoxy)-phenyl-triisopropylsilylacetyl-ene (**7**) (13.20g, 32.7mmol) was added to THF (50mL) and solution was cooled to 0°C. Tetrabutylammonium fluoride (38mL of 1M solution, 38mmol) was then added slowly to the solution. The solution was removed from the ice bath and stirred at room temperature for 70 minutes. The solution was then poured into 300mL of saturated ammonium chloride solution, and extracted twice with diethyl ether (150mL). The organic layer was dried with sodium sulfate. Flash column (silica; 100% hexane to 12% ethyl acetate in hexane gradient) gave 7.45g of product **8** (~92%).



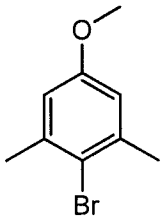
9

[0070] $Pd_2(dba)_3$ (250mg) and CuI (250mg) were added to 1,4-dioxane (20mL). The mixture was degassed for 20 minutes, $P(t\text{-}Bu)_3$ (12mL; solution as 10% in hexanes) was added, and degassing continued for 10 minutes. 3, 5-dimethyl-1-(2-(2-methoxyethoxy)ethoxy)-phenylacetylene (**8**) (4.0g, 16.1mmol) and 4-bromo-2,6-difluorobenzenonitrile (2.98g, 13.7mmol) were then added, and degassing continued for another 10 minutes. Diisopropylamine (7.2mL) was then added, and the reaction mixture was further degassed for 20 minutes. The reaction mixture was then heated at 68°C overnight under argon. The mixture was then cooled and poured into THF (200mL), filtered, and the solids were washed with additional THF. The combined filtrates were purified by flash column (silica; 5% to 30% ethyl acetate in hexane gradient) to give 4.44 g of product **9** (84% yield).

Scheme 3

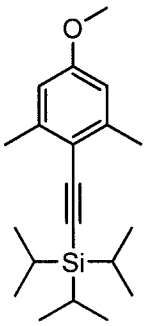


Example 2



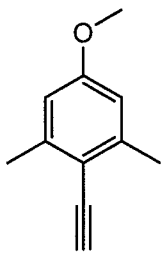
10

[0071] A mixture of 4-bromo-3, 5-dimethylphenol (4.0g, 19.9mmol) and K_2CO_3 (4.14g, 30.0mmol) was stirred in DMF (15mL) for 10 minutes. Iodomethane (5.76g, 40.0mmol) was added and the reaction mixture was heated at 35°C for 23 hours under argon. After cooling, the mixture was poured into DCM (150mL) and white solids were filtered off. Filtrate was purified by flash column (silica; 100% hexane) to give 2.79g of product **10** (65% yield).



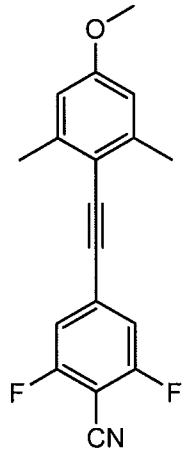
11

[0072] $Pd_2(dba)_3$ (150mg) and CuI (150mg) were added to 1,4-dioxane (15mL). The mixture was degassed for 20 minutes, 2, 6-dimethyl-4-methoxybromobenzene (**10**) (2.60g, 12.1mmol) and triisopropylsilylacetylene (9.43g, 51.7mmol) were added, and degassing continued for 10 minutes. Diisopropylamine (4.5mL) was then added, and the reaction mixture was degassed for 20 minutes. The mixture was heated at 90°C overnight under argon, cooled, and then poured into diethyl ether (100mL) and filtered. Flash column (silica; 100% hexane) gave 3.59g of product **11** (94% yield).



12

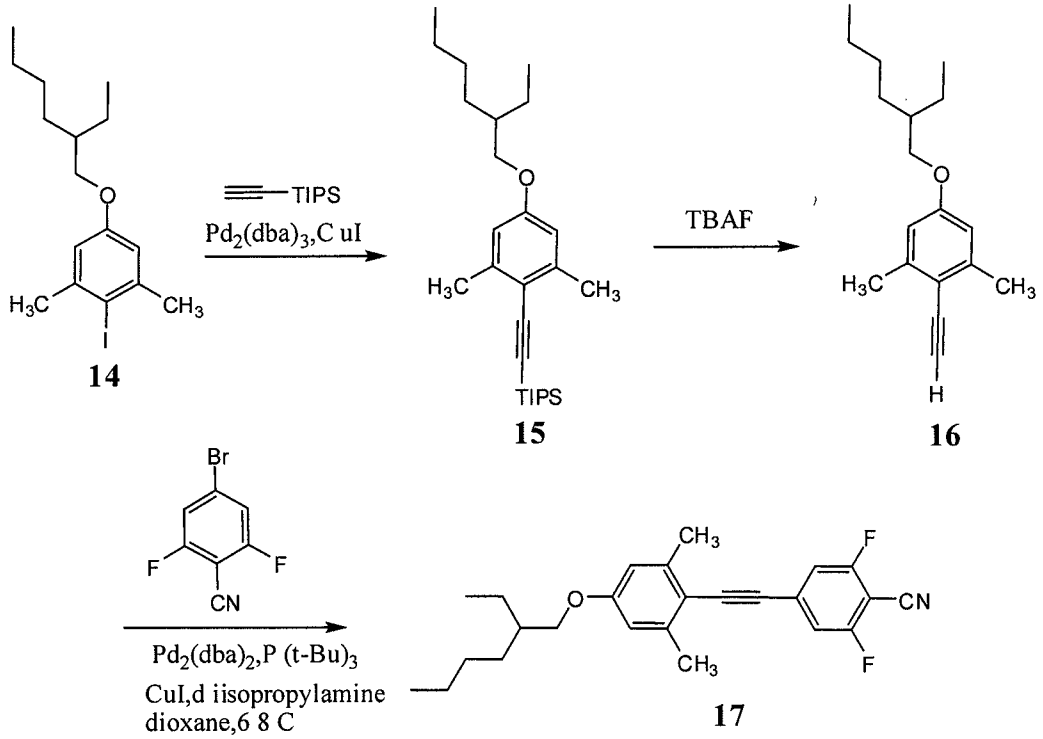
[0073] 3, 5-dimethyl-1-methoxyphenyltriisopropylacetylene (**11**) (3.50g, 11.1mmol) in THF (20mL) was cooled to 0°C, and tetrabutylammonium fluoride (15mL of 1M solution, 15mmol) was slowly added. The solution was removed from ice bath, stirred at room temperature for 60 minutes under argon, and then poured into 300mL of saturated ammonium chloride solution, and extracted twice with diethyl ether (100mL). Flash column (silica; 100% hexane) gave 1.47g of product **12** (83% yield).



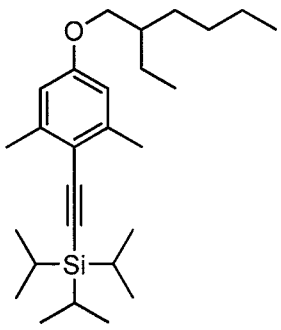
13

[0074] $Pd_2(dba)_3$ (100mg) and CuI (100mg) were added to 1,4-dioxane (15mL). The mixture was degassed for 20 minutes, $P(t\text{-}Bu)_3$ (4mL; solution as 10% in hexanes) was added, and degassing continued 10 minutes. 3, 5-dimethyl-1-methoxyphenylacetylene (**12**) (1.4g, 8.8mmol) and 4-bromo-2, 6-difluorobenzenonitrile (1.74g, 8.0mmol) were then added and degassing continued for 10 min. Diisopropylamine (2.5mL) was then added and the reaction mixture was degassed an additional 20 minutes. The mixture was then heated at 68°C overnight under argon. The mixture was then cooled, poured it into THF (150mL), and filtered. The filtrate was purified by flash column (silica; 100% hexane to 4% ethyl acetate in hexane gradient) to give 1.96g of crude material. After vacuum sublimation, 1.65g of product **13** was isolated (69% yield).

Scheme 4

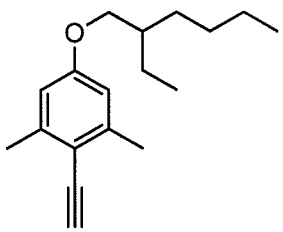


Example 3



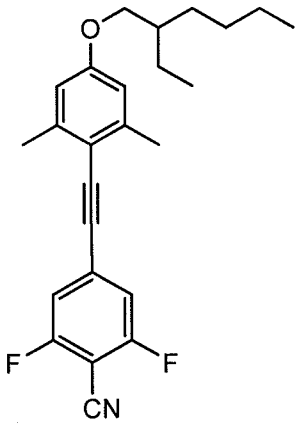
15

[0075] $Pd_2(dba)_3$ (100mg) and CuI (100mg) were added to 1,4-dioxane (15mL), and the mixture was degassed for 20 minutes. P(t-Bu)$_3$ (4mL; solution as 10% in hexanes) was then added, and degassing continued 10 minutes. Next, 2,6-dimethyl-4-(2-ethylhexoxy)iodobenzene (**14**) (1.5g, 4.2mmol) and triisopropylsilylacetylene (3.04g, 16.7mmol) were added and degassing continued 10 minutes. Finally, diisopropylamine (2.5mL) was added and reaction mixture was degassed for 20 minutes. The mixture was then heated at 90°C overnight under argon. After cooling, the reaction mixture was poured into diethyl ether (100mL) and filtered. Filtrate was purified by flash column (silica; 100% hexane) to give 1.52g of product **15** (88% yield).



16

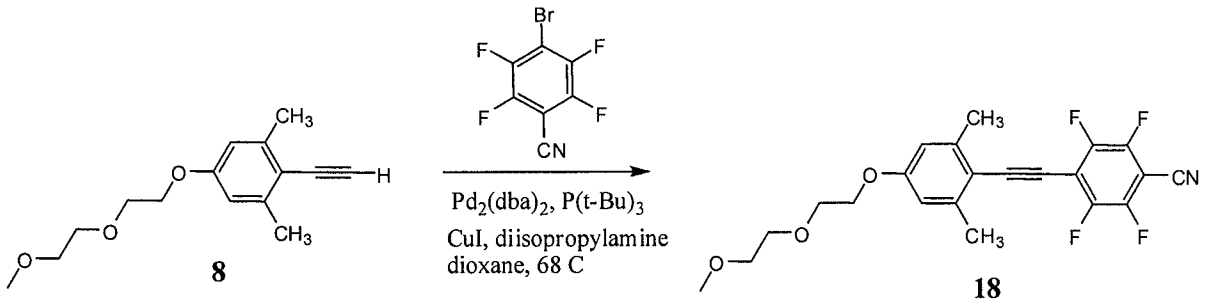
[0076] 3, 5-dimethyl-1-(2-ethylhexoxy)phenyltriisopropylsilylacetylene (**15**) (1.45g, 3.50 mmol) in THF (10mL) was cooled to 0°C, and tetrabutylammonium fluoride (4ml of 1M solution, 4mmol) was slowly added. The solution was then removed from the ice bath and stirred at room temperature for 60 minutes under argon. The solution was then poured into 150mL of saturated ammonium chloride solution and extracted with diethyl ether (3x 100mL). Flash column (silica; 100% hexane) gave 800mg of product **16** (84% yield).



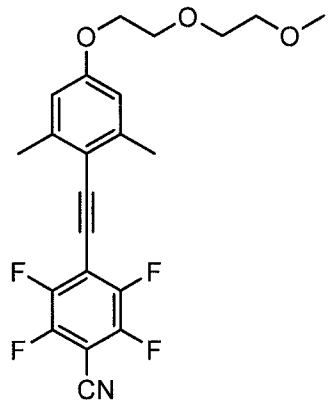
17

[0077] $Pd_2(dba)_3$ (70mg) and CuI (70mg) were added to 1,4-dioxane (15mL), and the mixture was degassed for 20 minutes. $P(t\text{-}Bu)_3$ (3mL; solution as 10% in hexanes) was then added, and degassing continued 10 minutes. 3, 5-dimethyl-1-(2-ethylhexoxy)phenylacetylene (**16**) (790mg, 2.7mmol) and 4-bromo-2, 6-difluorobenzenonitrile (525mg, 2.4mmol) were then added and degassing continued for 10 minutes. Diisopropylamine (2mL) was then added and the reaction mixture was degassed for 20 minutes. Next, the mixture was heated at 68°C overnight under argon. After cooling, the reaction mixture was poured into THF (100mL) and filtered. Filtrate was purified by flash column (silica; 2% to 25% DCM in hexane gradient). Recrystallization in DCM / MeOH gave 730mg of product **17** (74% yield).

Scheme 5



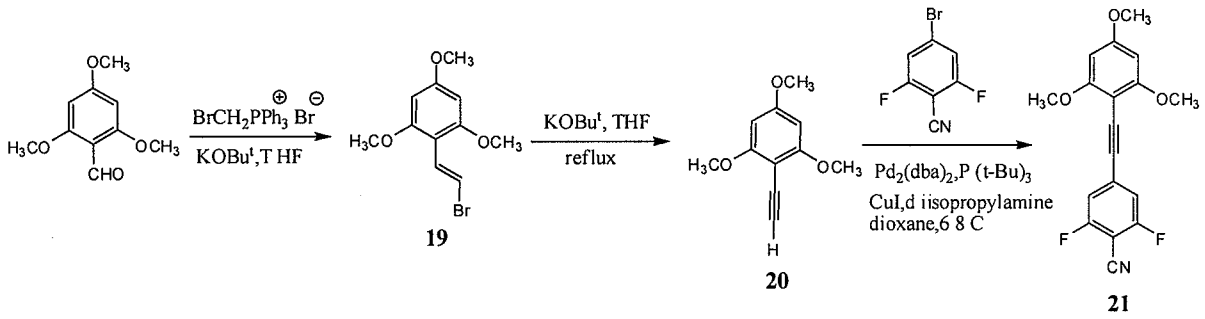
Example 4



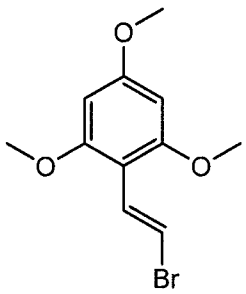
18

[0078] $Pd_2(dba)_3$ (75mg) and CuI (75mg) were added to 1,4-dioxane (20mL), and the mixture was degassed for 20 minutes. $P(t\text{-}Bu)_3$ (3mL; solution as 10% in hexanes) was then added, and degassing continued 10 minutes. 3, 5-dimethyl-1-(2-(2-methoxyethoxy)ethoxy)-phenylacetylene (**8**) (1.0g, 4.0mmol) and 4-bromo-2, 3, 5, 6-tetrafluorobenzenonitrile (886mg, 3.5mmol) were then added, degassing was continued for 10 minutes. Diisopropylamine (2mL) was then added, and the reaction mixture was further degassed for 20 minutes. The reaction mixture was then heated at 68°C overnight under argon. After heating, the mixture was cooled, then poured into THF (150mL) and filtered. Filtrate was purified by flash column (silica; 10% to 50% ethyl acetate in hexane gradient) to give 147mg of product **18** (9% yield).

Scheme 6

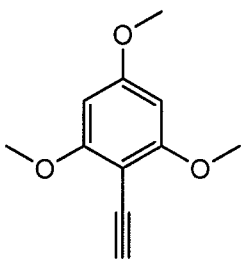


Example 5



19

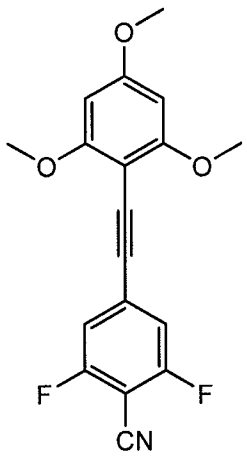
[0079] 2, 4, 6-trimethoxybenzaldehyde (10.0g, 51mmol) and bromomethyltriphenylphos-phonium bromide (24.45g, 56mmol) in THF (200mL) were cooled to 0°C, and potassium tert-butoxide (66mL of 1M solution, 66mmol) was slowly added. The reaction mixture was stirred overnight while slowly warming to room temperature. Flash column (silica; 10% to 20% ethyl acetate in hexane gradient) gave 9.3g of product **19** (67% yield).



20

[0080] 2-(2-bromoethenyl)-1, 3, 5-trimethoxybenzene (**19**) (9.27g, 33.9mmol) was dissolved in THF (200mL) and p otassium tert-butoxide (70mL of 1M solution, 70mmol) was slowly added. The reaction mixture was then heated under reflux (90°C) for two hours. After cooling, the KBr salt were filtered from the reaction mixture, and washed with additional THF (50mL). All filtrates were then combined, and purified by

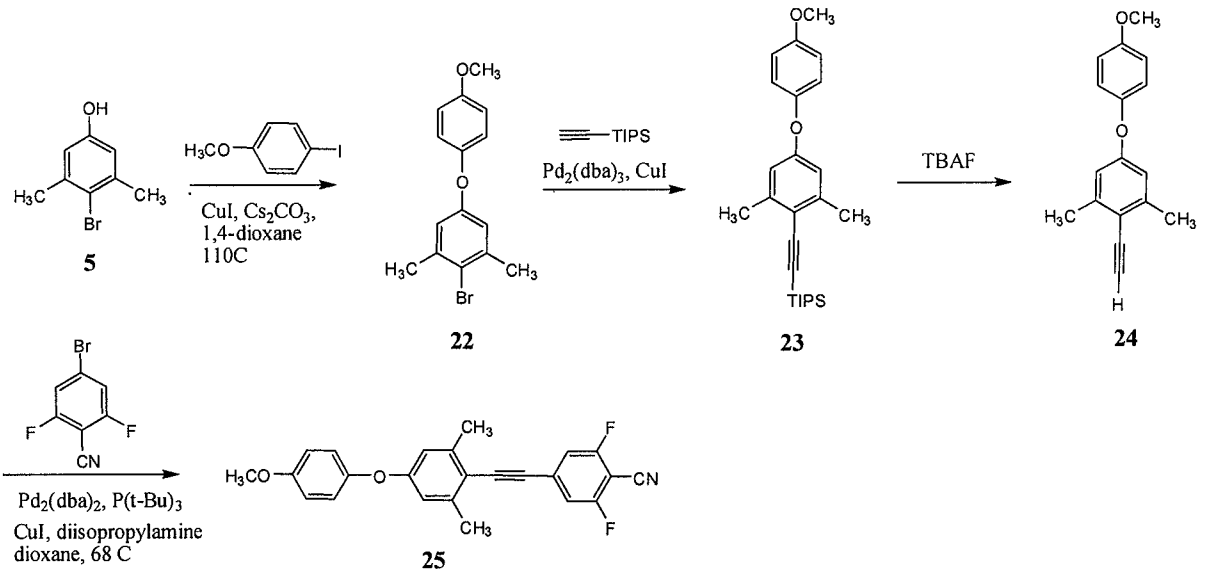
flash column (silica; 20% ethyl acetate in hexane) to give 3.84g of product **20** (59% yield).



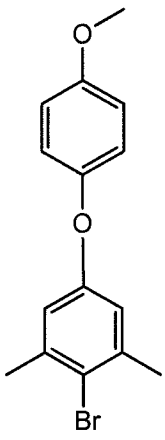
21

[0081] $Pd_2(dba)_3$ (150mg) and CuI (150mg) were added to 1,4-dioxane (30mL) and the mixture was degassed for 20 minutes. $P(t\text{-}Bu)_3$ (6mL; solution as 10% in hexanes) was then added, and degassing continued 10 minutes. 2, 4, 6-trimethoxyphenylacetylene (**20**) (2.0g, 10.4mmol) and 4-bromo-2, 6-difluorobenzenonitrile (2.13g, 9.8mmol) were next added and degassing continued for 10 minutes. Diisopropylamine (4.5mL) was then added, and reaction mixture was further degassed for 20 minutes. The reaction mixture was then heated at 68°C overnight under argon. After heating, the mixture was cooled, and then poured into THF (250mL) and filtered. A flash column done with the filtrate (silica; 10% to 50% ethyl acetate in hexane gradient) gave 1.45g of product **21** (45% yield).

Scheme 7

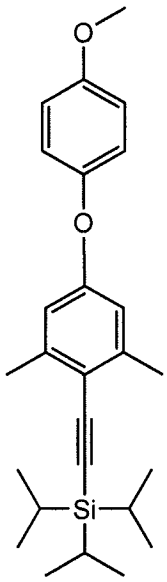


Example 6



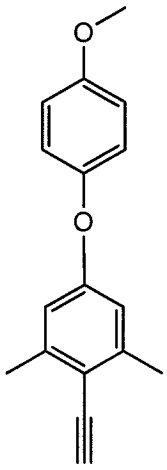
22

[0082] To a mixture of 4-iodoanisole (5.0g, 21.4mmol), 4-bromo-3, 5-dimethylphenol (6.44g, 32.1mmol), cesium carbonate (13.95g, 42.8mmol) and dimethylglycine hydrochloride (896mg, 6.42mmol) was added 1,4-dioxane (25mL). The freeze-thaw method (2 cycles) was used to purge the mixture. Copper Iodide (407mg, 2.14mmol) was then added to the mixture, and freeze-thaw (3 cycles) was continued. The reaction mixture was then heated at 120°C overnight. After cooling, the mixture was poured into ethyl acetate (200mL) and washed with water and brine. Flash column (silica; 100% hexane to 1% ethyl acetate in hexane gradient) gave 3.05g of product **22** (46% yield).



23

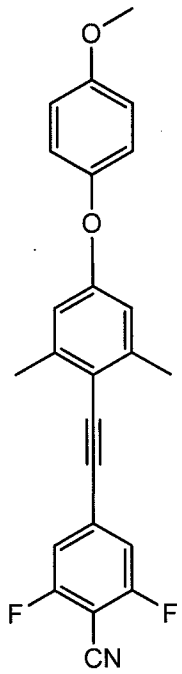
[0083] $Pd_2(dba)_3$ (250mg) and CuI (250mg) were added to 1,4-dioxane (35mL), and the mixture was degassed for 20 minutes. $P(t\text{-}Bu)_3$ (12mL; solution as 10% in hexanes) was added, and degassing continued 10 minutes. 1-Bromo-2, 6-dimethyl-4-(4-methoxyphenoxy)benzene (**22**) (3.90g, 12.66mmol) and triisopropylsilylacetylene (9.24g, 50.6mmol) were then added and degassing continued for 10 minutes. Diisopropylamine (7.5mL) was added next, and reaction mixture was further degassed for 20 minutes. The reaction mixture was then heated at 90°C overnight under argon. The mixture was cooled, then poured into diethyl ether (200mL) and filtered. A flash column of the filtrate (silica; 2% to 5% ethyl acetate in hexane gradient) gave 4.97g of product **23** (96% yield).



24

[0084] 2, 6-dimethyl-4-(4-methoxyphenoxy)phenyltriispropylsilylacetylene (**23**) (4.8g, 11.7 mmol) in THF (25mL) was cooled to 0°C, and tetrabutylammonium fluoride

(15mL of 1M solution, 15mmol) was slowly added. The solution was then removed from the ice bath and stirred at room temperature for 1.5 hours. After stirring, the solution was poured into saturated ammonium chloride solution (250mL) and extracted with diethyl ether (3 times 150mL). Flash column (silica; 2% TO 5% ethyl acetate in hexane gradient) gave 2.22g of product **24** (75% yield).



25

[0085] $Pd_2(dba)_3$ (150mg) and CuI (150mg) were added to 1,4-dioxane (20mL) and the mixture was degassed for 20 minutes. $P(t\text{-}Bu)_3$ (6mL; solution as 10% in hexanes) was then added, and degassing continued for 10 minutes. Next, 2, 6-dimethyl-4-(4-methoxyphenoxy)phenylacetylene (**24**) (1.5g, 5.9mmol) and 4-bromo-2, 6-difluorobenzenonitrile (1.18g, 5.4mmol) were added and degassing was continued for 10 minutes. Diisopropylamine (4.5mL) was then added, and reaction mixture was further degassed for 20 minutes. The reaction mixture was then heated at 68°C overnight under argon. After heating, the mixture was cooled, then poured into THF (200mL) and filtered. A flash column of the filtrate(silica; 2% to 10% ethyl acetate in hexane gradient) and two recrystallizations in DCM / hexane and DCM / MeOH gave 1.58g of product **25** (75% yield).

Example 7: Device Fabrication

[0086] Fabrication of light-emitting device: the ITO coated glass substrates were cleaned by ultrasound in acetone, and consecutively in 2-propanol, baked at 110°C

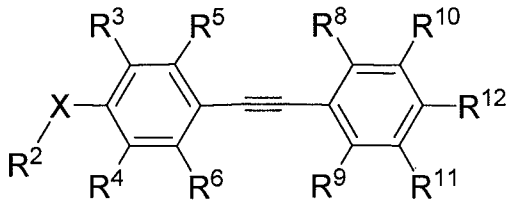
for 3 hours, followed by treatment with oxygen plasma for 5 min. A layer of PEDOT: PSS (Baytron P purchased from H.C. Starck) was spin-coated at 3000 rpm onto the pre-cleaned and O_2-plasma treated (ITO)-substrate and annealed at 180 °C for 10 min, yielding a thickness of around 40 nm. In a glove-box hosted vacuum deposition system at a pressure of 10^{-7} torr (1 torr=133.322 Pa), 4,4'4"-tri (N-carbazolyl)triphenylamine (TCTA) was first deposited on top of PEDOT/PSS layer at deposition rate of 0.06 nm/s, yielding a 30 nm thick film. Then 4,4'-bis(carbazol-9-yl)biphenyl (CBP) and deep blue emitter compound **9** were concurrently heated and deposited on top of TCTA under different deposition speed to make **9** at 3 wt%, followed by deposition of 1,3,5-tris(N-phenylbenzimidizol-2-yl)benzene (TPBI) at deposition rate around 0.06 nm/s. CsF and Al were then deposited successively at deposition rates of 0.005 and 0.2 nm/s, respectively. Each individual device has areas of 0.14 cm^2.

Example 8: Device Performance

[0087] Device A, comprising Compound 9 and fabricated in accordance with Examples 1 and 2, was tested to determine the emissive qualities of the device by examining the (1) emissive intensity of Device A (intensity of the device [a.u.] as a function of wavelength; (2) determining the CIE coordinates of Device A; and (3) determining the efficiency of Device A (current density and luminescence as a function of the voltage applied to the device; and external quantum efficiency and luminescence as a function of current density). All spectra were measured with an Ocean Optics HR 4000 spectrometer (Ocean Optics, Dunedin, FLA, USA) and I-V-L characteristics were taken with a Keithley 2400 SourceMeter (Keithley Instruments, Inc., Cleveland, OH, USA) and Newport 2832-C power meter and 818 UV detector (Newport, Corp., Irvine, CA, USA). All device operation was performed inside a nitrogen-filled glove-box. An exemplary configuration of the device (Device A) is shown in Figure 1. Figure 2 shows electroluminescence spectrum of Device A, plus the CIE coordinate. The spectrum shows significant emission between 400 and 500 nm. The purity of the deep blue emitted radiation is demonstrated by the CIE coordinates (X=0.16; Y = 0.10). In addition, as shown in Figures 3 and 4, Device A demonstrates efficacy in conventional organic light emitting device parameters. Thus Compound 9 has demonstrated its effectiveness as a blue emitting compound in organic light emitting devices.

WHAT IS CLAIMED IS:

1. A compound represented by a formula:



;

wherein R^2 is C_{1-30} alkyl, or $C_{1-30}O_{1-15}$ ether;

R^3, R^4, R^5, and R^6 are independently selected from –H, –F, –Cl, –Br, –I, C_{1-10} alkyl, $C_{1-10}O$ ether, and optionally substituted C_{6-10} aryl; provided that if R^2 is linear alkyl, at least one of R^3, R^4, R^5, and R^6 is not –H;

X is –O- or $-NR^7-$, wherein R^7 is –H, C_{1-12} alkyl, or $C_{1-12}O_{1-6}$ ether;

R^8 and R^9 are independently —H, –F, –Cl, –Br, –I, C_{1-10} alkyl or C_{1-10} ether; and

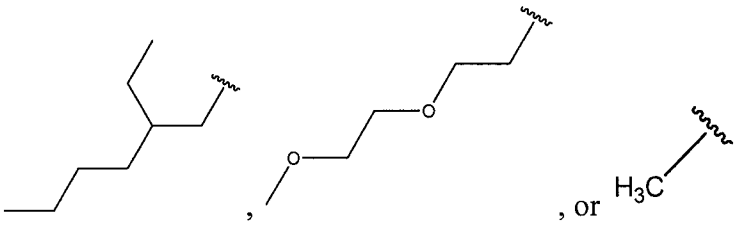
R^{10}, R^{11} and R^{12} are independently halogen, –CN, or $-NO_2$.

2. The compound of claim 1, wherein R^{12} is -CN.

3. The compound of claim 1 or 2, wherein R^{10} and R^{11} are –F.

4. The compound of any one of claims 1-3, wherein R^2 is C_{1-12} alkyl or $C_{1-9}O_{1-4}$ ether.

5. The compound of any one of claims 1-4 wherein R^2 is

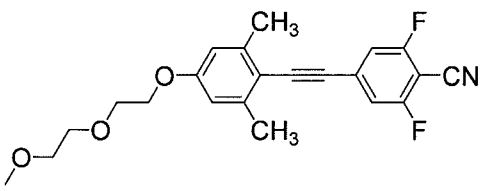


, or .

6. The compound of any one of claims 1-5, wherein R^3, R^4, R^5, and R^6 are independently selected from: -H, -F, -Cl, -Br, -I, C_{1-4} alkyl, and $C_{1-4}O$ ether.

7. The compound of any one of claims 1-6, wherein R^5 and R^6 are independently –CH_3, isopropyl, or -OCH_3.

8. The compound of any one of claims 1-7 selected from:



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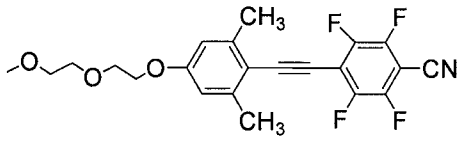

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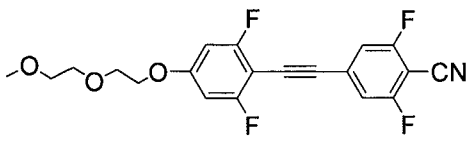
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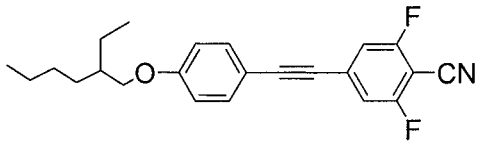
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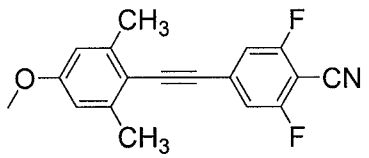
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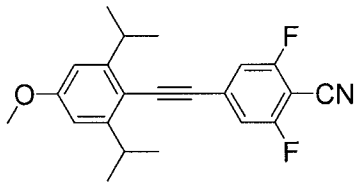
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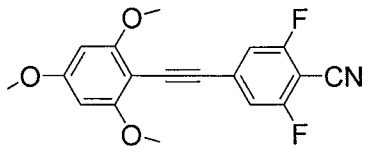
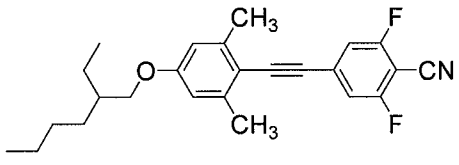

, and

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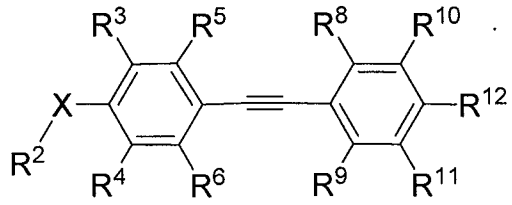
9. A light-emitting device, comprising:

an anode layer;

a cathode layer; and

a light-emitting layer positioned between the anode layer and the cathode layer, the light-emitting layer comprising a compound represented by a formula:


,

wherein R^2 is C_{1-30} alkyl, or $C_{1-30}O_{1-15}$;

R^3, R^4, R^5, and R^6 are independently selected from –H, -F, -Cl, -Br, -I, C_{1-10} alkyl, $C_{1-10}O$ ether, and optionally substituted C_{6-10} aryl; provided that if R^2 is methyl, ethyl, propyl, or isopropyl, at least one of R^3, R^4, R^5, and R^6 is not –H;

X is –O- or $-NR^7-$;

R^7 is wherein R^7 is –H, C_{1-12} alkyl, or $C_{1-12}O_{1-6}$ ether;

R^8 and R^9 are independently –H, -F, -Cl, -Br, -I, C_{1-10} alkyl or C_{1-10} ether; and

R^{10}, R^{11} and R^{12} are independently halogen, -CN, or $-NO_2$.

10. The device of claim 9 wherein R^{10} and R^{11} are independently –F, -Cl, or -Br.

11. The device of any one of claims 9-10 wherein R^{12} is -CN.

12. The device of any one of claims 9-11, wherein if R^2 is alkyl, at least one of R^3, R^4, R^5, and R^6 is not –H.

13. The device of any one of claims 9-12, wherein R^2 is C_{4-30} alkyl.

14. The device of any one of claims 9-12, wherein R^2 is $C_{1-9}O_{1-4}$ ether.

15. The device of any one of claims 9-14, wherein X is –O-.

16. The device of any one of claims 9-14, wherein X is $–NR^7-$.

FIG. 1

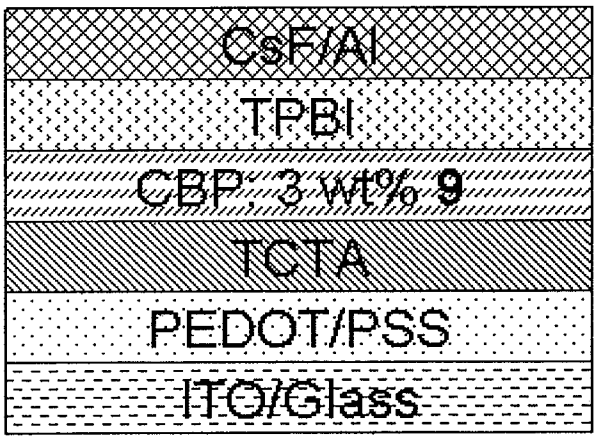


FIG. 2

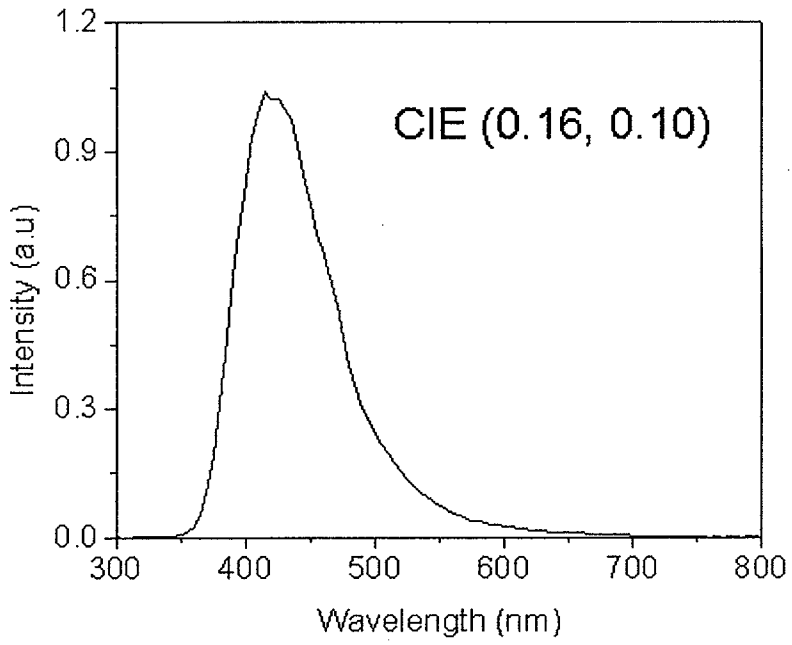

CIE (0.16, 0.10)
Intensity (a.u)
Wavelength (nm)
0.0
0.3
0.6
0.9
1.2
300
400
500
600
700
800

FIG. 3

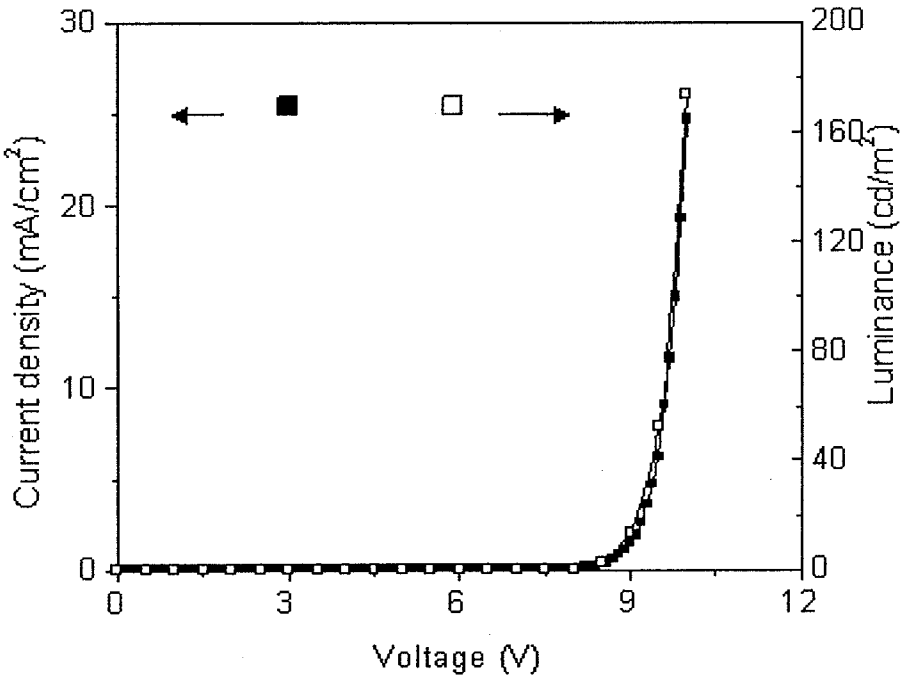
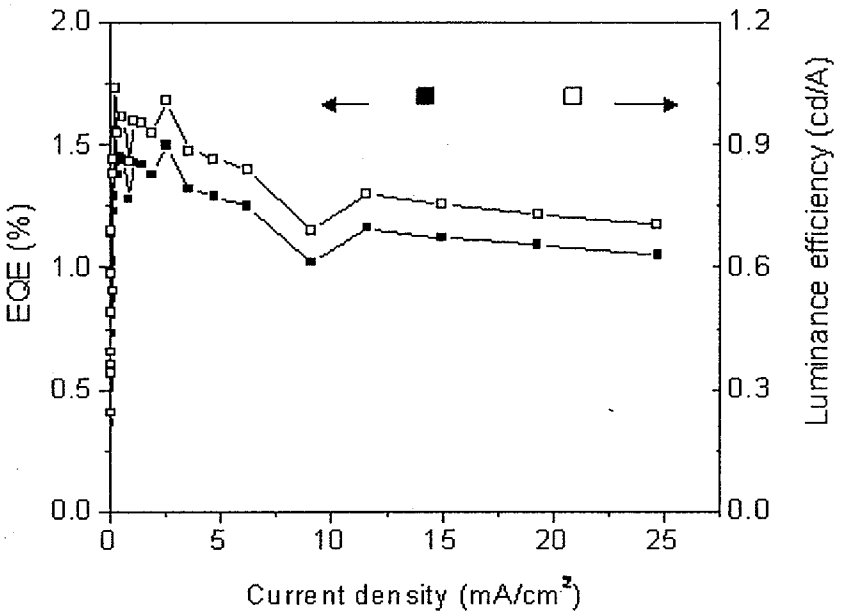

30
20
10
0
0
3
6
9
12
200
160
120
80
40
0
Current density (mA/cm^2)
Luminance (cd/m^2)
Voltage (V)

FIG. 4


2.0
1.5
1.0
0.5
0.0
EQE (%)
1.2
0.9
0.6
0.3
0.0
Luminance efficiency (cd/A)
0
5
10
15
20
25
Current density (mA/cm²)

INTERNATIONAL SEARCH REPORT

International application No
PCT/US2010/037301

A. CLASSIFICATION OF SUBJECT MATTER
INV. C09K11/06 H05B33/14 C07C255/50 H01L51/50
ADD.

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
C09K H05B C07C H01L

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, WPI Data, CHEM ABS Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	GB 2 367 057 A (MERCK PATENT GMBH [DE]) 27 March 2002 (2002-03-27)	1-4
A	* page 22, Example 15 *	9-16
X	CN 1 293 180 A (SHANGHAI INST ORGANIC CHEM [CN]) 2 May 2001 (2001-05-02)	1,3-6
A	* page 9, Scheme 7, second compound *	9-16
X	JP 8 184865 A (TOYO INK MFG CO) 16 July 1996 (1996-07-16)	1,4,6
A	* page 5, Table 1, compound G *	9-16
A	WO 02/093244 A2 (MERCK PATENT GMBH [DE]; HECKMEIER MICHAEL [DE]; GOETZ ACHIM [DE]) 21 November 2002 (2002-11-21) the whole document	1-16

☐ Further documents are listed in the continuation of Box C.

☒ See patent family annex.

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"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
26 July 2010	04/08/2010

Name and mailing address of the ISA/	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Nemes, Csaba A.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/US2010/037301

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
GB 2367057 A	27-03-2002	NONE	
CN 1293180 A	02-05-2001	NONE	
JP 8184865 A	16-07-1996	NONE	
WO 02093244 A2	21-11-2002	AU 2002342821 A1	25-11-2002
		DE 10217273 A1	05-12-2002
		JP 2005504993 T	17-02-2005
		JP 2009282534 A	03-12-2009
		US 2004150633 A1	05-08-2004