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(54) **ORGANIC LIGHT EMITTING HOST MATERIALS**

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USPC **257/40; 544/405**

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(57) **ABSTRACT**

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Heteroaryl-aryl compounds such as compounds represented by Formula may be used in electronic devices such as organic light-emitting devices. For example, the compounds may be used as an emissive material in an emissive layer.

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FIG.1

LiF(1 nm)/Al (100nm)
TPBI (40nm)
BE-2 (5 nm)
BE- 2:lr(piq)2acac
BE-2 (5nm)
DTASI (30 nm)
PEDOT (30 nm)
ITO (55 nm)

FIG.2

ORGANIC LIGHT EMITTING HOST MATERIALS

BACKGROUND

[0001] 1. Field

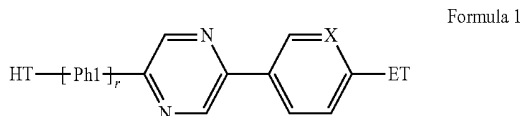
[0002] The embodiments relate to emissive compounds for light-emitting layers in devices.

[0003] 2. Description of the Related Art

[0004] Organic light-emitting devices (OLED) are becoming increasingly important in lighting and display applications. OLEDs may include an emissive or light-emitting layer that includes a host material and an emissive component dispersed within the host material. Emissive materials of OLED devices may have problems with low stability. This potential deficiency with emissive materials may contribute to low efficiency and short lifetime of the devices comprising the emissive materials.

SUMMARY

[0005] Some embodiments include an emissive compound of formula:



wherein, HT is optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine, wherein Ph¹ is a p-phenylene, wherein ET is optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzthiazol-2-yl, wherein X is CH or N, and wherein r is 1, 2, 3.

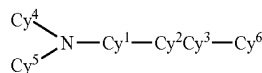
[0006] With respect to Formula 1, in some embodiments, HT is unsubstituted diphenylamine, a mono-substituted diphenylamine, a di-substituted diphenylamine, an unsubstituted phenyl(naphthyl)amine, a mono-substituted phenyl(naphthyl)amine, and/or an unsubstituted carbazolyl. In some embodiments, ET is an unsubstituted benzoimidazol-2-yl.

[0007] Some embodiments include a compound represented by Formula 1a:



wherein HT is optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine; each Ph¹ is independently optionally substituted p-phenylene, wherein the p-phenylene directly bonded to HT may optionally form a bond to a phenyl of HT to form a three ring system; Py is optionally substituted pyrazin-2,5-ylene; Het is optionally substituted p-phenylene or optionally substituted pyridin-2,5-ylene; ET is optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzothiazol-2-yl; and r is 1, 2, or 3.

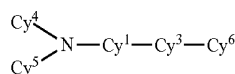
[0008] Some embodiments include a compound represented by Formula 2:



wherein Cy¹ is a p-phenylene optionally substituted with 1 or 2 substituents independently selected from C₁₋₆ alkyl and F; Cy² is independently a 2,5-pyridyl optionally substituted with 1, 2, or 3 substituents independently selected from C₁₋₆ alkyl and F, or a pyrazine optionally substituted with 1, 2, or 3 substituents independently selected from C₁₋₆ alkyl and F; Cy³ is pyridin-2,5-ylene optionally substituted with 1, 2, or 3 substituents independently selected from C₁₋₆ alkyl and F, or a p-phenylene optionally substituted with 1 or 2 substituents independently selected from C₁₋₆ alkyl and F; Cy⁴ and Cy⁵ are independently optionally substituted phenyl or optionally substituted naphthyl, wherein Cy⁴ and Cy⁵ may be joined to form, with the nitrogen atom to which they are attached, a carbazolyl ring system; and Cy⁶ is 1-phenyl-1H-benzo[d]imidazol-2-yl optionally substituted with 1, 2, 3, 4, or 5 substituents independently selected from C₁₋₆ alkyl and F.

[0009] With respect to Formula 2, in some embodiments Cy¹, and Cy² are independently p-phenylene optionally substituted with 1 or 2 substituents independently selected from C₁₋₆ alkyl and F; Cy⁴ is phenyl optionally substituted with 1, 2, or 3 substituents independently selected from C₁₋₆ alkyl and F; Cy⁵ is phenyl optionally substituted with 1, 2, or 3 substituents independently selected from C₁₋₆ alkyl and F, or a naphth-1-yl or naphth-2-yl optionally substituted with 1, 2, or 3 substituents independently selected from C₁₋₆ alkyl and F; and Cy⁶ is 1-phenyl-1H-benzo[d]imidazol-2-yl optionally substituted with 1, 2, 3, 4, or 5 substituents independently selected from C₁₋₆ alkyl and F.

[0010] Some embodiments include a compound represented by Formula 3:



wherein Cy¹ is an optionally substituted p-phenylene; Cy³ is selected from an optionally substituted 2,5-pyrazine-3'-pyridine, and optionally substituted 2,5-pyrazine-2',5'-phenyl, an optionally substituted 2,5-bi-pyridinyl, an optionally substituted 3,3'-bi-pyridinyl, and an optionally substituted 3,2':5',3''-terpyridinyl; Cy⁴ and Cy⁵ are optionally substituted phenyl or optionally substituted naphthyl; and Cy⁶ is optionally substituted 1-phenyl-1H-benzo[d]imidazol-2-yl.

[0011] With respect to Formula 3, in some embodiments Cy¹ is an optionally substituted interphenylene, independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy³ is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy⁴ is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy⁵ is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl; wherein Cy⁶ is independently optionally substituted with H, F, methyl, ethyl, propyl, or isopropyl.

[0012] Some embodiments include optionally substituted [(para-phenylenyl-para-azolyl)]compounds, including optionally substituted N,N-diphenyl-4-(6-(1-phenyl-1H-

benzo[d]imidazol-2-yl)pyridin-3-yl)aniline; N-phenyl-N-(4'-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)-[1,1'-biphenyl]-4-yl)naphthalen-1-amine; 4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-N,N-di-p-tolyl-[1,1'-biphenyl]-4-amine; 9,9-dimethyl-N,N-diphenyl-7-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-9H-fluoren-2-amine; N,N-diphenyl-4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-[1,1'-biphenyl]-4-amine; 4-methyl-N-(4-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)phenyl)-N-(p-tolyl)aniline; N-phenyl-N-(4-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)phenyl)naphthalen-1-amine; 9,9-dimethyl-7-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,3'-bipyridin]-6-yl)-N,N-di-p-tolyl-9H-fluoren-2-amine; N,N-diphenyl-4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-[1,1'-biphenyl]-4-amine; 4'-(3-methyl-6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-N,N-diphenyl-[1,1'-biphenyl]-4-amine; N-phenyl-N-(4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-[1,1'-biphenyl]-4-yl)naphthalen-2-amine; N-phenyl-N-(4'-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)-[1,1'-biphenyl]-4-yl)naphthalen-1-amine; 4-methyl-N-(4-(6'-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[2,3'-bipyridin]-5-yl)phenyl)-N-(p-tolyl)aniline; N,N-diphenyl-4-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)-[3,2':5',3"-terpyridin]-6"-yl)aniline, etc.

[0013] Some embodiments include a light-emitting device comprising a compound described herein.

[0014] These and other embodiments are described in more detail herein. These and other embodiments are described in more detail herein.

BRIEF DESCRIPTION OF THE DRAWINGS

[0015] FIG. 1 is a schematic drawing of an embodiment of an OLED device comprising a compound disclosed herein.

[0016] FIG. 2 is a schematic drawing of an embodiment of an OLED device described in Example 2.

DETAILED DESCRIPTION

[0017] Unless otherwise indicated, when a compound or chemical structural feature such as aryl is referred to as being "optionally substituted," it is meant that the feature may have no substituents (i.e. be unsubstituted) or may have one or more substituents. A feature that is "substituted" has one or more substituents. The term "substituent" has the ordinary meaning known to one of ordinary skill in the art. In some embodiments, the substituent may be an ordinary organic moiety known in the art, which may have a molecular weight (e.g. the sum of the atomic masses of the atoms of the substituent) of 15 g/mol to 50 g/mol, 15 g/mol to 100 g/mol, 15 g/mol to 200 g/mol, 15 g/mol to 300 g/mol, or 15 g/mol to 500 g/mol. In some embodiments, the substituent comprises: 0-30, 0-20, 0-10, or 0-5 carbon atoms; and 0-30, 0-20, 0-10, or 0-5 heteroatoms independently selected from: N, O, S, Si, F, Cl, Br, or I; provided that the substituent comprises at least one atom selected from: C, N, O, S, Si, F, Cl, Br, or I. Examples of substituents include, but are not limited to, alkyl, alkenyl, alkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, aryl, heteroaryl, hydroxy, alkoxy, aryloxy, acyl, acyloxy, alkylcarboxylate, thiol, alkylthio, cyano, halo, thiocarbonyl, O-carbamyl, N-carbamyl, O-thiocarbamyl, N-thiocarbamyl,

C-amido, N-amido, S-sulfonamido, N-sulfonamido, isocyanato, thiocyanato, isothiocyanato, nitro, silyl, sulfonyl, sulfanyl, sulfonyl, haloalkyl, haloalkoxy, trihalomethanesulfonyl, trihalomethanesulfonamido, amino, etc. In some embodiments, two substituents may combine to form a ring.

[0018] As used herein the term "alkyl" has the broadest meaning generally understood in the art, and may include a moiety composed of carbon and hydrogen containing no double or triple bonds. Alkyl may be linear alkyl, branched alkyl, cycloalkyl, or a combination thereof, and in some embodiments, may contain from one to thirty-five carbon atoms. In some embodiments, alkyl may include C₁₋₁₀ linear alkyl, such as methyl (—CH₃), ethyl (—CH₂CH₃), n-propyl (—CH₂CH₂CH₃), n-butyl (—CH₂CH₂CH₂CH₃), n-pentyl (—CH₂CH₂CH₂CH₂CH₃), n-hexyl (—CH₂CH₂CH₂CH₂CH₂CH₃), etc.; C₃₋₁₀ branched alkyl, such as C₃H₇ (e.g. iso-propyl), C₄H₉ (e.g. branched butyl isomers), C₅H₁₁ (e.g. branched pentyl isomers), C₆H₁₃ (e.g. branched hexyl isomers), C₇H₁₅ (e.g. heptyl isomers), etc.; C₃₋₁₀ cycloalkyl, such as C₃H₅ (e.g. cyclopropyl), C₄H₇ (e.g. cyclobutyl isomers such as cyclobutyl, methylcyclopropyl, etc.), C₅H₉ (e.g. cyclopentyl isomers such as cyclopentyl, methylcyclobutyl, dimethylcyclopropyl, etc.) C₆H₁₁ (e.g. cyclohexyl isomers), C₇H₁₃ (e.g. cycloheptyl isomers), etc.; and the like.

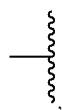
[0019] As used herein, the term "alkoxy" includes —O-alkyl, such as —OCH₃, —OC₂H₅, —OC₃H₇ (e.g. propoxy isomers such as isopropoxy, n-propoxy, etc.), —OC₄H₉ (e.g. butoxy isomers), —OC₅H₁₁ (e.g. pentoxy isomers), —OC₆H₁₃ (e.g. hexoxy isomers), —OC₇H₁₅ (e.g. heptoxy isomers), etc.

[0020] With respect to an optionally substituted moiety such as optionally substituted alkyl, a phrase such as "optionally substituted C₁₋₁₂ alkyl" refers to a C₁₋₁₂ alkyl that may be unsubstituted, or may have 1 or more substituents, and does not limit the number of carbon atoms in any substituent. A phrase such as "C₁₋₁₂ optionally substituted alkyl" refers to unsubstituted C₁₋₁₂ alkyl, or substituted alkyl wherein both the alkyl parent and all substituents have from 1-12 carbon atoms. Similar conventions may be applied to other optionally substituted moieties such as aryl and heteroaryl.

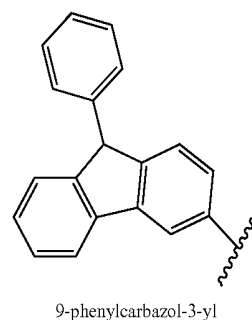
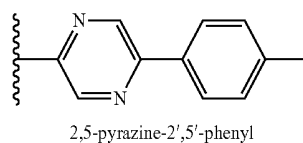
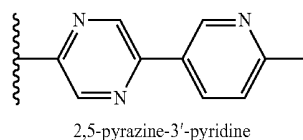
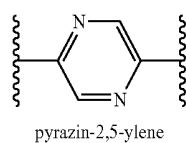
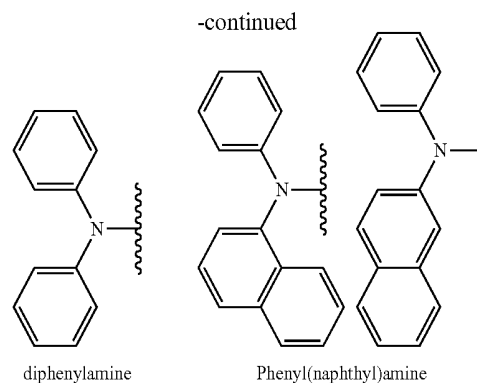
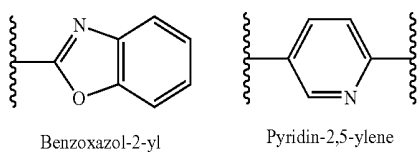
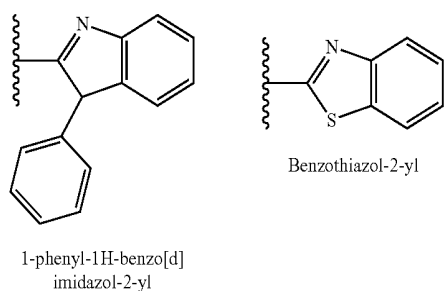
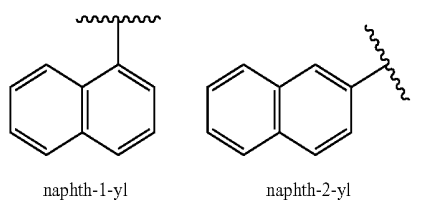
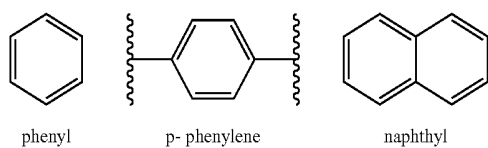
[0021] Substituents on alkyl may be the same as those described generally above, except that alkyl may not have an alkyl substituent. In some embodiments, substituents on alkyl are independently selected from F, Cl, Br, I, CN, CO₂H, —O-alkyl, ester groups, acyl, amine groups, and amide groups, and may have a molecular weight of about 15 to about 100 or about 500.

[0022] For convenience, the term "molecular weight" is used with respect to a moiety or part of a molecule to indicate the sum of the atomic masses of the atoms in the moiety or part of a molecule, even though it may not be a complete molecule.

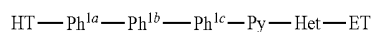
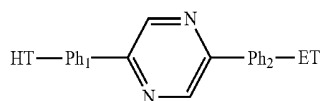
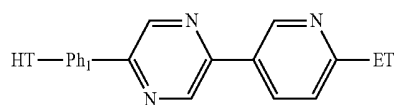
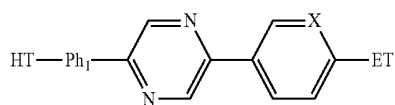
[0023] The structures associated with some of the chemical names referred to herein are depicted below. These structures may be unsubstituted, as shown below, or a substituent may independently be in any position normally occupied by a hydrogen atom when the structure is unsubstituted. Unless a point of attachment is indicated by

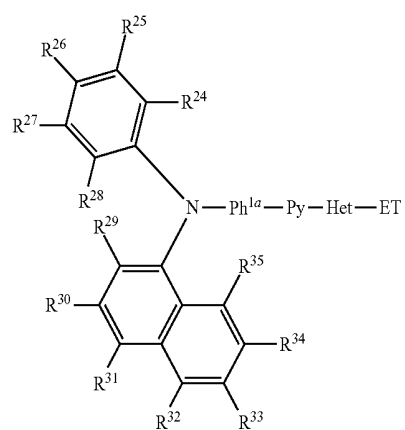
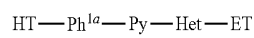


attachment may occur at any position normally occupied by a hydrogen atom.



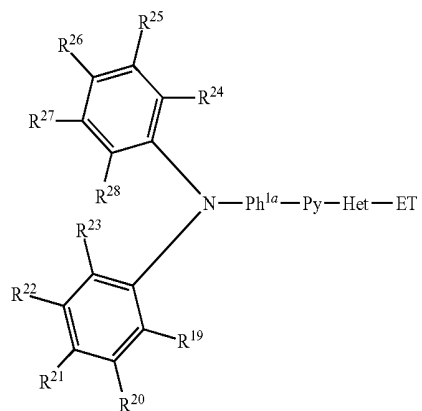
[0024] In some embodiments, a compound is provided represented by the following formulae:





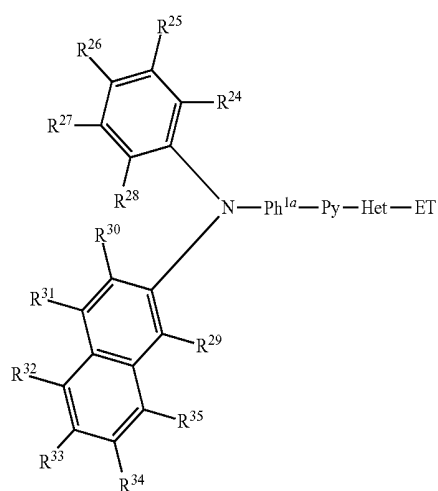
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Formula 8

Formula 9



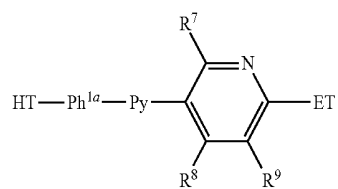
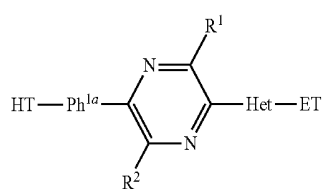
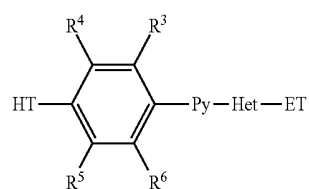
Formula 10

Formula 11



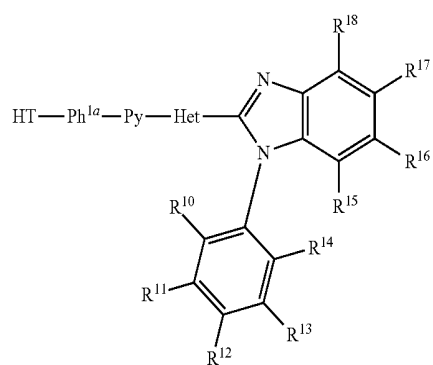
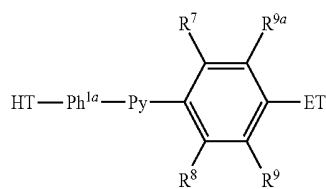
Formula 12

Formula 13



Formula 14

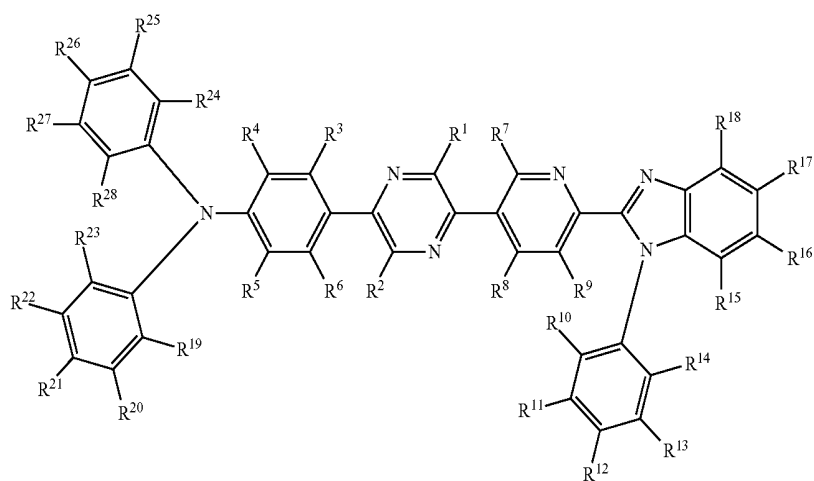
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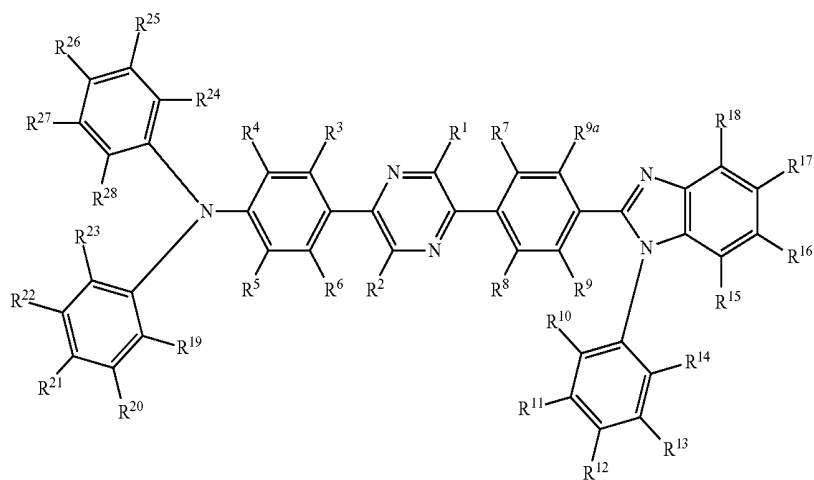
Formula 16

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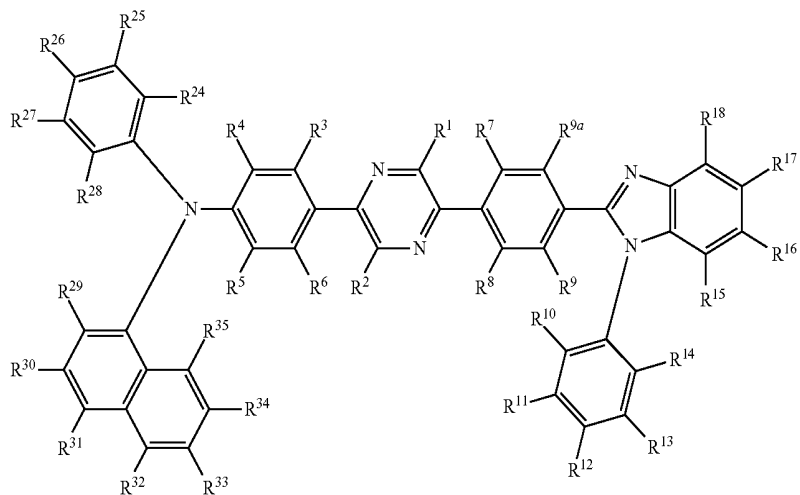
Formula 17



Formula 18

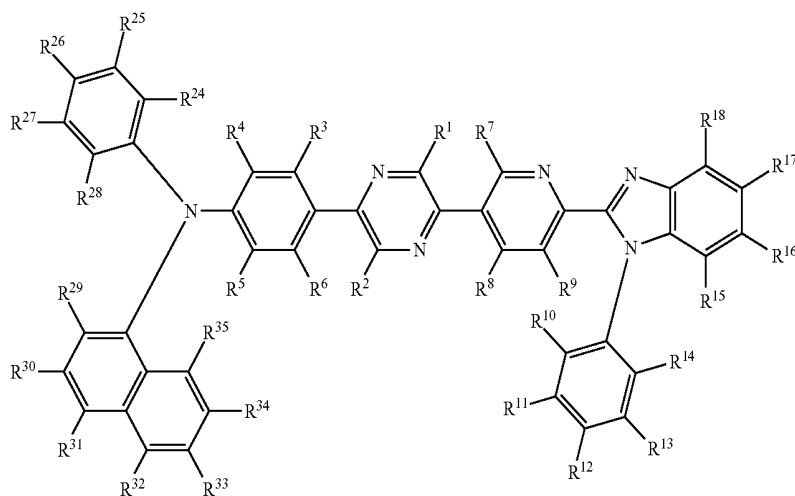


Formula 19

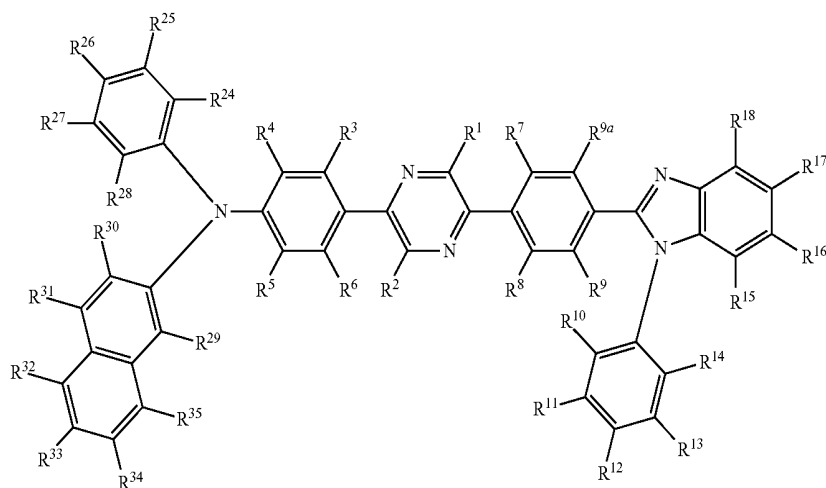


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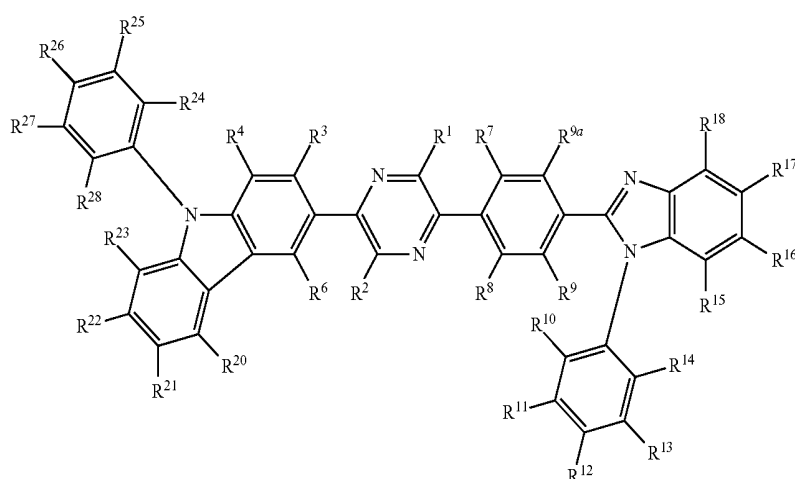
Formula 20



Formula 21



Formula 22

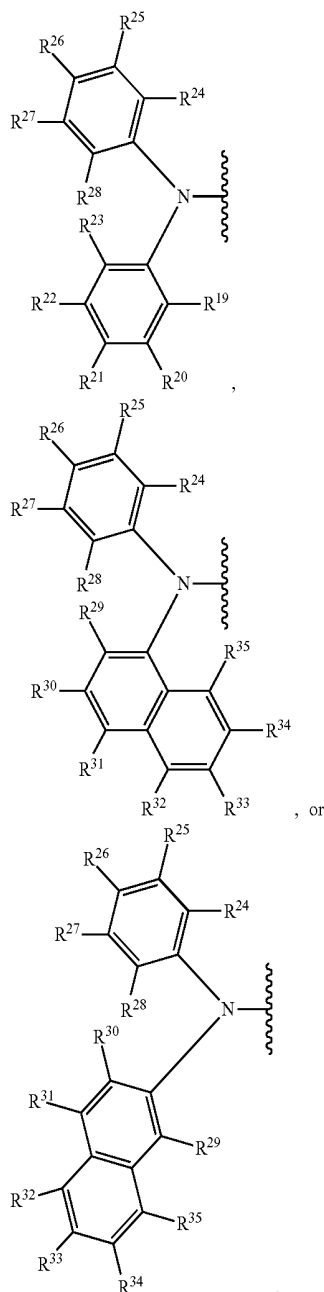


[0025] With respect to any relevant formula or structural representation herein, HT may be optionally substituted diphenylamine or optionally substituted phenyl(naphthyl) amine. If the diphenylamine is substituted, it may have 1, 2, 3, 4, 5, 6, 7, 8, 9, or 10 substituents. In some embodiments, the diphenylamine may have 1, 2, 3, or 4 substituents, or 1 or 2 substituents. If the phenyl(naphthyl)amine is substituted, it

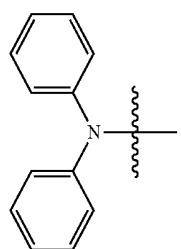
may have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12 substituents. In some embodiments, the phenyl(naphthyl)amine may have 1, 2, 3, or 4 substituents, or 1 or 2 substituents. In some embodiments, some or all of the substituents on HT may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or

a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C₁₋₁₀ optionally substituted alkyl, such as CH₃, C₂H₅, C₃H₇, cyclic C₃H₅, C₄H₉, cyclic C₄H₇, C₅H₁₁, cyclic C₅H₉, C₆H₁₃, cyclic C₆H₁₁, etc., which may be optionally substituted; C₁₋₁₀ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO₂; C₁₋₆ fluoroalkyl, such as CF₃, CF₂H, C₂F₅, etc.; a C₁₋₁₀ ester such as —O₂CCH₃, —CO₂CH₃, —O₂CC₂H₅, —CO₂C₂H₅, —O₂C-phenyl, —CO₂-phenyl, etc.; a C₁₋₁₀ ketone such as —COCH₃, —COC₂H₅, —COC₃H₇, —CO-phenyl, etc.; or C₁₋₁₀ amino such as NH₂, NH(CH₃), N(CH₃)₂, N(CH₃)C₂H₅, etc. In some embodiments, any substituents on HT can be an electron donating substituent, such as C₁₋₃ alkyl, C₁₋₃—O-alkyl, NH₃, or C₁₋₃ amino. In some embodiments, HT is unsubstituted.

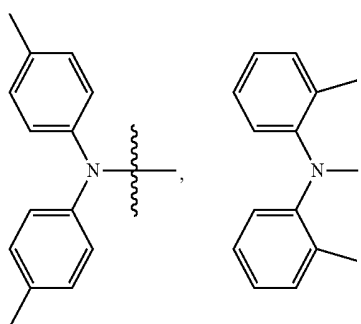
[0026] In some embodiments, HT is:



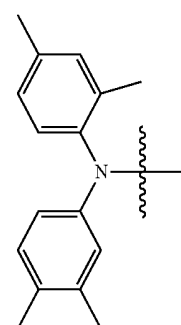
[0027] In some embodiments, HT can be selected from optionally substituted carbazolyl, optionally substituted diphenylamine and/or optionally substituted phenyl(naphthyl)amine with 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11 or 12 substituents independently selected from C₁₋₆ alkyl and F. In some embodiments, HT is selected from unsubstituted diphenylamine, a mono-substituted diphenylamine, a di-substituted diphenylamine, an unsubstituted phenyl(naphthyl)amine, a mono-substituted phenyl(naphthyl)amine, and/or an unsubstituted carbazolyl. Examples of the described ring systems may include any one of the following:



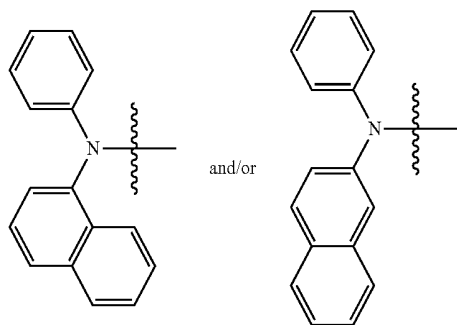
unsubstituted diphenylamine



a mono-substituted diphenylamine

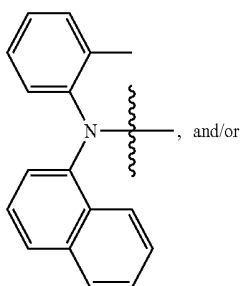


a di-substituted diphenylamine

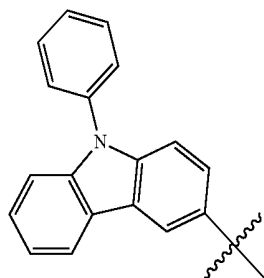


an unsubstituted phenyl(naphthyl)amine

-continued

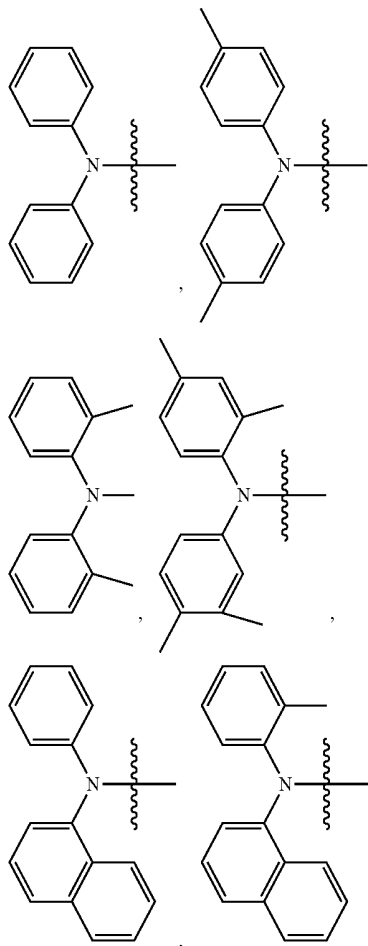


a mono-substituted phenyl(naphthyl)amine,

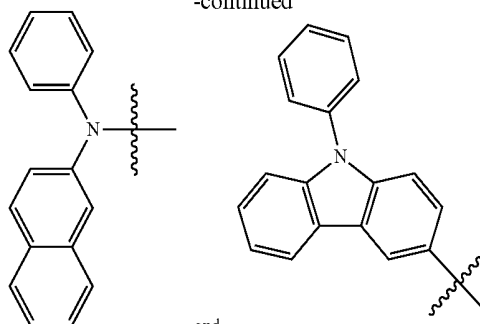


an unsubstituted carbazoyl

[0028] In some embodiments, HT is selected any one of



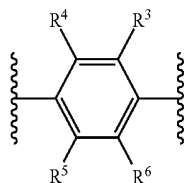
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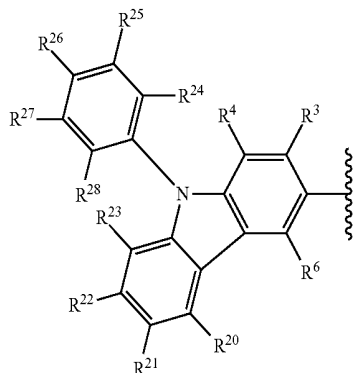
, and

[0029] With respect to any relevant formula or structural representation herein, Ph^{1a} may be optionally substituted p-phenylene, or HT-Ph^{1a} may be 9-phenylcarbazol-3-yl. If the p-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the p-phenylene is unsubstituted. In some embodiments the p-phenylene has 1 substituent. In some embodiments, the p-phenylene has 2 substituents. In some embodiments the p-phenylene has 3 substituents. In some embodiments the p-phenylene has 4 substituents. If the 9-phenylcarbazol-3-yl is substituted, it may have it may have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, or 11, or 12 substituents. In some embodiments, the 9-phenylcarbazol-3-yl may have 1, 2, 3, or 4 substituents, or 1 or 2 substituents. In some embodiments, some or all of the substituents on Ph^{1a} or HT-Ph^{1a} may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C_{1-10} optionally substituted alkyl, such as CH_3 , C_2H_5 , C_3H_7 , cyclic C_3H_5 , C_4H_9 , cyclic C_4H_7 , C_5H_{11} , cyclic C_5H_9 , C_6H_{13} , cyclic C_6H_{11} , etc., which may be optionally substituted; C_{1-10} optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO_2 ; C_{1-6} fluoroalkyl, such as CF_3 , CF_2H , C_2F_5 , etc.; a C_{1-10} ester such as $-\text{O}_2\text{CCH}_3$, $-\text{CO}_2\text{CH}_3$, $-\text{O}_2\text{CC}_2\text{H}_5$, $-\text{CO}_2\text{C}_2\text{H}_5$, $-\text{O}_2\text{C-phenyl}$, $-\text{CO}_2\text{-phenyl}$, etc.; a C_{1-10} ketone such as $-\text{COCH}_3$, $-\text{COC}_2\text{H}_5$, $-\text{COC}_3\text{H}_7$, $-\text{CO-phenyl}$, etc.; or C_{1-10} amino such as NH_2 , $\text{NH}(\text{CH}_3)$, $\text{N}(\text{CH}_3)_2$, $\text{N}(\text{CH}_3)\text{C}_2\text{H}_5$, etc. In some embodiments, any substituents on Ph^{1a} or HT-Ph^{1a} can be C_{1-3} alkyl, C_{1-3} -O-alkyl, NH_3 , or C_{1-3} amino. In some embodiments, Ph^{1a} or HT-Ph^{1a} is unsubstituted.

[0030] In some embodiments, Ph^{1a} is:



[0031] In some embodiments, HT-Ph^{1a} is:



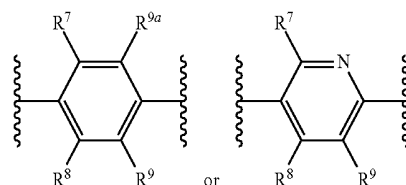
[0032] With respect to any relevant formula or structural representation herein, Ph^{1b} may be a bond or optionally substituted p-phenylene. If the p-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the p-phenylene is unsubstituted. In some embodiments the p-phenylene has 1 substituent. In some embodiments, the p-phenylene has 2 substituents. In some embodiments the p-phenylene has 3 substituents. In some embodiments the p-phenylene has 4 substituents. In some embodiments, some or all of the substituents on Ph^{1b} may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C₁₋₁₀ optionally substituted alkyl, such as CH₃, C₂H₅, C₃H₇, cyclic C₃H₅, C₄H₉, cyclic C₄H₇, C₅H₁₁, cyclic C₅H₉, C₆H₁₃, cyclic C₆H₁₁, etc., which may be optionally substituted; C₁₋₁₀ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO₂; C₁₋₆ fluoroalkyl, such as CF₃, CF₂H, C₂F₅, etc.; a C₁₋₁₀ ester such as —O₂CCH₃, —CO₂CH₃, —O₂CC₂H₅, —CO₂C₂H₅, —O₂C-phenyl, —CO₂-phenyl, etc.; a C₁₋₁₀ ketone such as —COCH₃, —COC₂H₅, —COC₃H₇, —CO-phenyl, etc.; or C₁₋₁₀ amino such as NH₂, NH(CH₃), N(CH₃)₂, N(CH₃)C₂H₅, etc. In some embodiments, any substituents on Ph^{1b} can be C₁₋₃ alkyl, CF₃, or F. In some embodiments, Ph^{1b} is a bond.

[0033] With respect to any relevant formula or structural representation herein, Ph^{1c} may be a bond or optionally substituted p-phenylene. If the p-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the p-phenylene is unsubstituted. In some embodiments the p-phenylene has 1 substituent. In some embodiments, the p-phenylene has 2 substituents. In some embodiments the p-phenylene has 3 substituents. In some embodiments the p-phenylene has 4 substituents. In some embodiments, some or all of the substituents on Ph^{1c} may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C₁₋₁₀ optionally substituted alkyl, such as CH₃, C₂H₅, C₃H₇, cyclic C₃H₅, C₄H₉, cyclic C₄H₇, C₅H₁₁, cyclic C₅H₉, C₆H₁₃, cyclic C₆H₁₁, etc., which may be optionally substituted; C₁₋₁₀ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO₂; C₁₋₆ fluoroalkyl, such as CF₃, CF₂H, C₂F₅, etc.; a C₁₋₁₀ ester such as —O₂CCH₃, —CO₂CH₃, —O₂CC₂H₅, —CO₂C₂H₅, —O₂C-phenyl,

—CO₂-phenyl, etc.; a C₁₋₁₀ ketone such as —COCH₃, —COC₂H₅, —COC₃H₇, —CO-phenyl, etc.; or C₁₋₁₀ amino such as NH₂, NH(CH₃), N(CH₃)₂, N(CH₃)C₂H₅, etc. In some embodiments, any substituents on Ph^{1c} can be C₁₋₃ alkyl, CF₃, or F. In some embodiments, Ph^{1c} is a bond.

[0034] With respect to any relevant formula or structural representation herein, Py may be optionally substituted pyrazin-2,5-ylene. If the pyrazin-2,5-ylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the pyrazin-2,5-ylene is unsubstituted. In some embodiments the pyrazin-2,5-ylene has 1 substituent. In some embodiments, the pyrazin-2,5-ylene has 2 substituents. In some embodiments, some or all of the substituents on Py may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C₁₋₁₀ optionally substituted alkyl, such as CH₃, C₂H₅, C₃H₇, cyclic C₃H₅, C₄H₉, cyclic C₄H₇, C₅H₁₁, cyclic C₅H₉, C₆H₁₃, cyclic C₆H₁₁, etc., which may be optionally substituted; C₁₋₁₀ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO₂; C₁₋₆ fluoroalkyl, such as CF₃, CF₂H, C₂F₅, etc.; a C₁₋₁₀ ester such as —O₂CCH₃, —CO₂CH₃, —O₂CC₂H₅, —CO₂C₂H₅, —O₂C-phenyl, —CO₂-phenyl, etc.; a C₁₋₁₀ ketone such as —COCH₃, —COC₂H₅, —COC₃H₇, —CO-phenyl, etc.; or C₁₋₁₀ amino such as NH₂, NH(CH₃), N(CH₃)₂, N(CH₃)C₂H₅, etc. In some embodiments, any substituents on Py can be C₁₋₃ alkyl, CF₃, or F. In some embodiments, Py is unsubstituted.

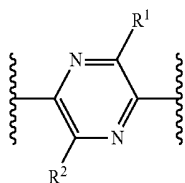
[0035] In some embodiments, Py is:



[0036] With respect to any relevant formula or structural representation herein, Het may be optionally substituted p-phenylene or optionally substituted pyridin-2,5-ylene. If the p-phenylene is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the p-phenylene is unsubstituted. In some embodiments the p-phenylene has 1 substituent. In some embodiments, the p-phenylene has 2 substituents. In some embodiments the p-phenylene has 3 substituents. In some embodiments the p-phenylene has 4 substituents. If the pyridin-2,5-ylene is substituted, it may have 1, 2, or 3 substituents. In some embodiments, the pyridin-2,5-ylene is unsubstituted. In some embodiments the pyridin-2,5-ylene has 1 substituent. In some embodiments, the pyridin-2,5-ylene has 2 substituents. In some embodiments the pyridin-2,5-ylene has 3 substituents. In some embodiments, some or all of the substituents on Het may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C₁₋₁₀ optionally substituted alkyl, such as CH₃, C₂H₅, C₃H₇, cyclic C₃H₅, C₄H₉, cyclic C₄H₇, C₅H₁₁, cyclic C₅H₉, C₆H₁₃, cyclic C₆H₁₁, etc., which may be optionally substituted; C₁₋₁₀ optionally substituted

tuted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO₂; C₁₋₆ fluoroalkyl, such as CF₃, CF₂H, C₂F₅, etc.; a C₁₋₁₀ ester such as —O₂CCH₃, —CO₂CH₃, —O₂CC₂H₅, —CO₂C₂H₅, —O₂C-phenyl, —CO₂-phenyl, etc.; a C₁₋₁₀ ketone such as —COCH₃, —COC₂H₅, —COC₃H₇, —CO-phenyl, etc.; or C₁₋₁₀ amino such as NH₂, NH(CH₃), N(CH₃)₂, N(CH₃)C₂H₅, etc. In some embodiments, any substituents on Het can be C₁₋₃ alkyl, CF₃, or F. In some embodiments, Het is unsubstituted.

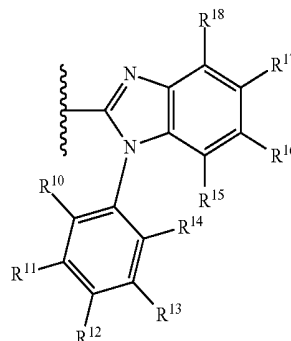
[0037] In some embodiments, Het is:



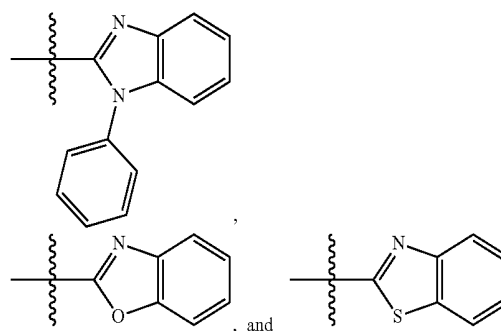
[0038] With respect to any relevant formula or structural representation herein, ET may be optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzothiazol-2-yl. If the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl is substituted, it may have 1, 2, 3, or 4 substituents. In some embodiments, the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl is unsubstituted. In some embodiments the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 1 substituent. In some embodiments, the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 2 substituents. In some embodiments the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 3 substituents. In some embodiments the benzimidazol-2-yl, benzoxazol-2-yl, or benzothiazol-2-yl has 4 substituents.

[0039] In some embodiments, ET is optionally substituted 1-phenyl-1H-benzo[d]imidazol-2-yl. In some embodiments, the 1-phenyl-1H-benzo[d]imidazol-2-yl is unsubstituted. If the 1-phenyl-1H-benzo[d]imidazol-2-yl is substituted, it can have 1, 2, 3, 4, 5, 6, 7, 8, or 9 substituents. In some embodiments, the 1-phenyl-1H-benzo[d]imidazol-2-yl has 1, 2, 3, or 4 substituents. In some embodiments, the 1-phenyl-1H-benzo[d]imidazol-2-yl has 1 or 2 substituents. In some embodiments, some or all of the substituents on ET may have: from 0 to 10 carbon atoms and from 0 to 10 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I (provided that there is at least 1 non-hydrogen atom); and/or a molecular weight of 15 g/mol to 500 g/mol. For example, the substituents may be C₁₋₁₀ optionally substituted alkyl, such as CH₃, C₂H₅, C₃H₇, cyclic C₃H₅, C₄H₉, cyclic C₄H₇, C₅H₁₁, cyclic C₅H₉, C₆H₁₃, cyclic C₆H₁₁, etc., which may be optionally substituted; C₁₋₁₀ optionally substituted alkoxy; halo, such as F, Cl, Br, I; OH; CN; NO₂; C₁₋₆ fluoroalkyl, such as CF₃, CF₂H, C₂F₅, etc.; a C₁₋₁₀ ester such as —O₂CCH₃, —CO₂CH₃, —O₂CC₂H₅, —CO₂C₂H₅, —O₂C-phenyl, —CO₂-phenyl, etc.; a C₁₋₁₀ ketone such as —COCH₃, —COC₂H₅, —COC₃H₇, —CO-phenyl, etc.; or C₁₋₁₀ amino such as NH₂, NH(CH₃), N(CH₃)₂, N(CH₃)C₂H₅, etc. In some embodiments, any substituents on ET can be C₁₋₃ alkyl, or an electron withdrawing substituent such as F, Cl, NO₂, CN, COH, COCH₃, etc. In some embodiments, ET is unsubstituted.

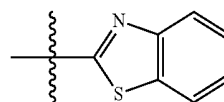
[0040] In some embodiments, ET is:



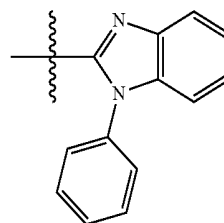
[0041] In some embodiments, ET can be selected from optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, and/or optionally substituted benzthiazol-2-yl. In some embodiments, ET is an unsubstituted benzoimidazol-2-yl. In some embodiments, ET is selected from



In some embodiments, ET is an optionally substituted benzimidazol-2-yl.



In some embodiments, ET is



[0042] With respect to any relevant formula above, Ph¹ and/or Ph² can be an optionally substituted p-phenylene.

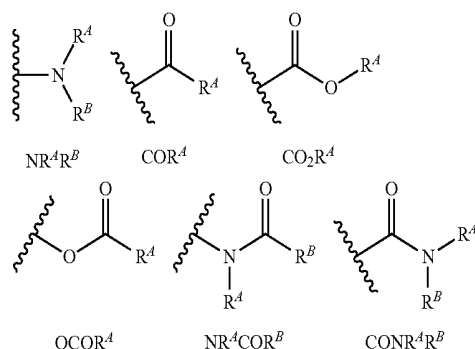
[0043] With respect to any relevant formula above, X can be selected from C and N, e.g., Formula 3 and/or 2 respectively.

[0044] In some embodiments, Ph¹ is optionally substituted p-phenylene with 1, 2, 3 or 4 substituents independently selected from C₁₋₆ alkyl and F. In some embodiments, Ph¹ is an unsubstituted p-phenylene.

[0045] In some embodiments, Ph² is optionally substituted p-phenylene with 1, 2, 3 or 4 substituents independently selected from C₁₋₆ alkyl and F. In some embodiments, Ph² is an unsubstituted p-phenylene.

[0046] Generally R¹-R³⁵, may be H or any substituent, such as a substituent having from 0 to 6 carbon atoms and from 0 to 5 heteroatoms, wherein each heteroatom is independently: O, N, S, F, Cl, Br, or I, and/or having a molecular weight of 15 g/mol to 300 g/mol. Any of R¹-R³⁵ may comprise: a) 1 or more alkyl moieties optionally substituted with, or optionally connected by or to, b) 1 or more functional groups, such as C=C, C≡C, CO, CO₂, CON, NCO₂, OH, SH, O, S, N, N=C, F, Cl, Br, I, CN, NO₂, CO₂H, NH₂, etc.; or may be a substituent having no alkyl portion, such as F, Cl, Br, I, NO₂, CN, NH₂, OH, COH, CO₂H, etc.

[0047] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R¹ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R¹ may be H; F; Cl; CN; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C₁₋₆ amino, such as —NHCH₃, —NH(CH₃)₂, —NHCH₂CH₃, etc.; C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc.; CHO; C₂₋₆—CO-alkyl, such as —COCH₃, —COC₂H₅, —COC₃H₇, COC₄H₉, —COC₅H₁₁, etc.; CO₂H; C₂₋₆—CO₂-alkyl, —CO₂CH₃, —CO₂C₂H₅, —CO₂C₃H₇, CO₂C₄H₉, —COC₅H₁₁, etc. In some embodiments, R¹ may be H.



[0048] Each R^A may independently be H, or C₁₋₁₂ alkyl, including: linear or branched alkyl having a formula C_aH_{a+1}, or cycloalkyl having a formula C_aH_{a-1}, wherein a is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12, such as linear or branched alkyl of a formula: CH₃, C₂H₅, C₃H₇, C₄H₉, C₅H₁₁, C₆H₁₃, C₇H₁₅, C₈H₁₇, C₉H₁₉, C₁₀H₂₁, etc., or cycloalkyl of a formula: C₃H₅, C₄H₇, C₅H₉, C₆H₁₁, C₇H₁₃, C₈H₁₅, C₉H₁₇, C₁₀H₁₉, etc. In some embodiments, R^A may be H or C₁₋₆ alkyl. In some

embodiments, R^A may be H or C₁₋₃ alkyl. In some embodiments, R^A may be H or CH₃. In some embodiments, R^A may be H.

[0049] Each R^B may independently be H, or C₁₋₁₂ alkyl, including: linear or branched alkyl having a formula C_aH_{a+1}, or cycloalkyl having a formula C_aH_a, wherein a is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, or 12, such as linear or branched alkyl of a formula: CH₃, C₂H₅, C₃H₇, C₄H₉, C₅H₁₁, C₆H₁₃, C₈H₁₇, C₇H₁₅, C₉H₁₉, C₁₀H₂₁, etc., or cycloalkyl of a formula: C₃H₅, C₄H₇, C₅H₉, C₆H₁₁, C₇H₁₃, C₈H₁₅, C₉H₁₇, C₁₀H₁₉, etc. In some embodiments, R^B may be H or C₁₋₃ alkyl. In some embodiments, R^B may be H or CH₃. In some embodiments, R^B may be H.

[0050] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R² may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R² may be H; F; Cl; CN; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C₁₋₆ amino, such as —NHCH₃, —NH(CH₃)₂, —NHCH₂CH₃, etc.; C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc.; CHO; C₂₋₆—CO-alkyl, such as —COCH₃, —COC₂H₅, —COC₃H₇, COC₄H₉, —COC₅H₁₁, etc.; CO₂H; C₂₋₆—CO₂-alkyl, —CO₂CH₃, —CO₂C₂H₅, —CO₂C₃H₇, CO₂C₄H₉, —COC₅H₁₁, etc. In some embodiments, R² may be H.

[0051] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³ may be H; F; Cl; CN; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C₁₋₆ amino, such as —NHCH₃, —NH(CH₃)₂, —NHCH₂CH₃, etc.; C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc.; CHO; C₂₋₆—CO-alkyl, such as —COCH₃, —COC₂H₅, —COC₃H₇, COC₄H₉, —COC₅H₁₁, etc.; CO₂H; C₂₋₆—CO₂-alkyl, —CO₂CH₃, —CO₂C₂H₅, —CO₂C₃H₇, CO₂C₄H₉, —COC₅H₁₁, etc. In some embodiments, R³ may be H.

[0052] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R⁴ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R⁴ may be H; F; Cl; CN; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; C₁₋₆ amino, such as —NHCH₃, —NH(CH₃)₂, —NHCH₂CH₃, etc.; C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pen-

—O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R²⁸ may be H.

[0081] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R²⁹ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R²⁹ may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R²⁹ may be H.

[0082] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³⁰ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³⁰ may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R³⁰ may be H.

[0083] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³¹ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³¹ may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R³¹ may be H.

[0084] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³² may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³² may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R³² may be H.

[0085] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³³ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³³ may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and

isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R³³ may be H.

[0086] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³⁴ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³⁴ may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R³⁴ may be H.

[0087] With respect to any relevant formula or structural depiction herein, some non-limiting examples of R³⁵ may include R^A, F, Cl, CN, OR^A, CF₃, NO₂, NR^AR^B, COR^A, CO₂R^A, OCORA, NR^ACOR^B, CONR^AR^B, etc. In some embodiments, R³⁵ may be H; F; Cl; CF₃; OH; NH₂; C₁₋₆ alkyl, such as methyl, ethyl, propyl isomers (e.g. n-propyl and isopropyl), cyclopropyl, butyl isomers, cyclobutyl isomers (e.g. cyclobutyl and methylcyclopropyl), pentyl isomers, cyclopentyl isomers, hexyl isomers, cyclohexyl isomers, etc.; or C₁₋₆ alkoxy, such as —O-methyl, —O-ethyl, isomers of —O-propyl, —O-cyclopropyl, isomers of —O-butyl, isomers of —O-cyclobutyl, isomers of —O-pentyl, isomers of —O-cyclopentyl, isomers of —O-hexyl, isomers of —O-cyclohexyl, etc. In some embodiments, R³⁵ may be H.

[0088] Some embodiments include optionally substituted N,N-diphenyl-4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)aniline. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0089] Some embodiments include optionally substituted 4-methyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(p-tolyl)aniline. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0090] Some embodiments include optionally substituted N-phenyl-N-(4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)phenyl)naphthalen-1-amine. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0091] Some embodiments include optionally substituted N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-1-amine. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0092] Some embodiments include optionally substituted 2-methyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)aniline. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0093] Some embodiments include optionally substituted N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)aniline. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

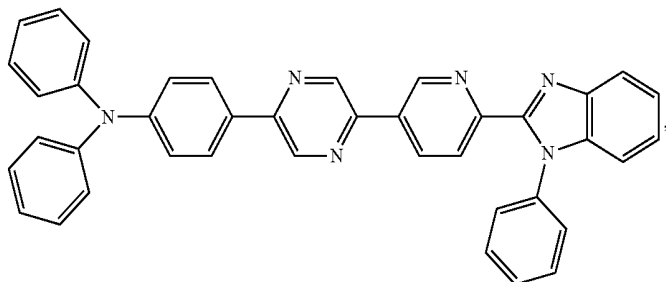
[0094] Some embodiments include optionally substituted N,N-diphenyl-4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)aniline. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0095] Some embodiments include optionally substituted N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

[0096] Some embodiments include optionally substituted N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-2-amine. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

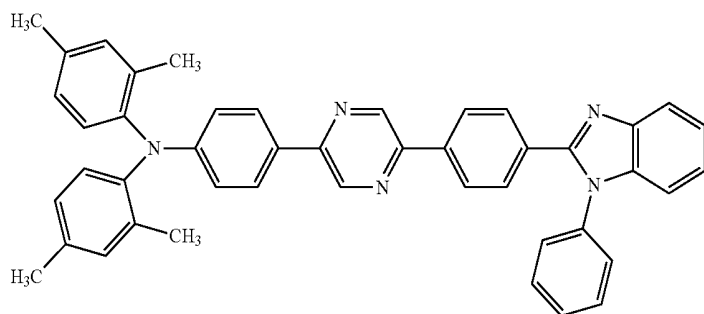
[0097] Some embodiments include optionally substituted 9-phenyl-3-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)-9H-carbazole. In some embodiments, any substituents may independently be CH₃, C₂H₅, C₃H₇, F, or CF₃. In some embodiments, the compound is unsubstituted.

(BE-1)



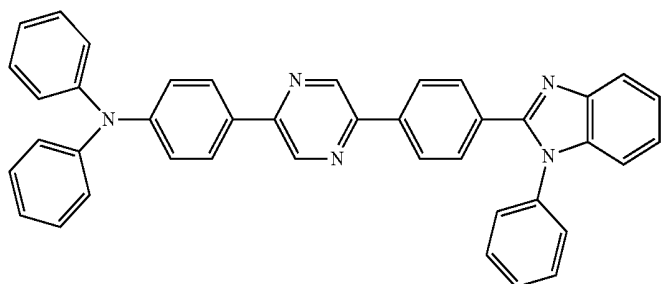
N,N-diphenyl-4-(5-(6-(1-phenyl-1H-benzo[d]imidazol-2-yl)pyridin-3-yl)pyrazin-2-yl)aniline

(BE-6)



N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)aniline

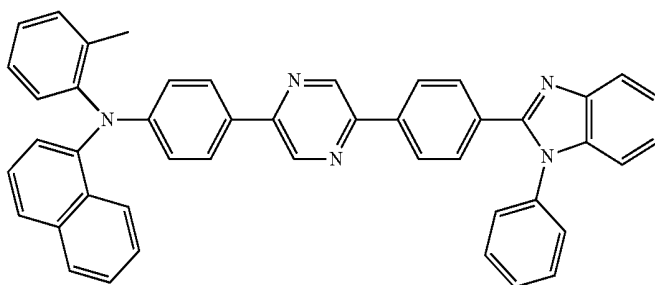
(BE-7)



N,N-diphenyl-4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)aniline

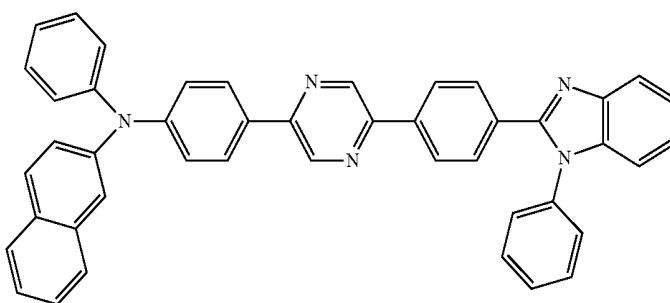
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(BE-8)



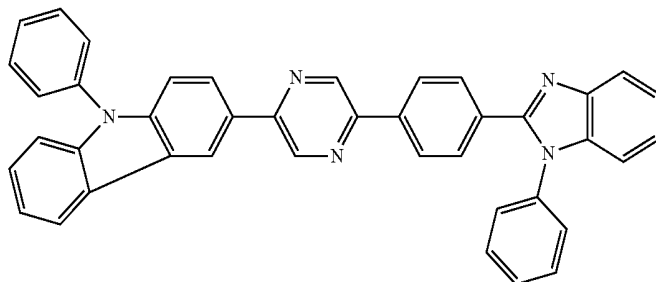
N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine

(BE-9)



N-phenyl-N-(4-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)phenyl)naphthalen-2-amine

(BE-10)



9-phenyl-3-(5-(4-(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl)pyrazin-2-yl)-9H-carbazole

[0098] In some embodiments, a compound of any of the formulae, structures and/or names above (hereinafter referred to as "a subject compound") may be electroluminescent, or may be fluorescent or phosphorescent. In some embodiments, the compound has fluorescence in the blue or violet visible light range or phosphorescence in the red, orange, yellow, and/or green visible light range. In some embodiments, the compound may have a lowest energy triplet state with an energy over than about 2.5 eV, such as about 2.5 eV to about 4 eV, about 2.5 eV to about 3.5 eV, or about 3 eV to about 3.5 eV.

[0099] In some embodiments, a light-emitting device is provided, comprising a compound described above.

[0100] In some embodiments, a light emitting device is provided, wherein the compound is an emissive material in an emissive layer.

[0101] Some embodiments include a composition comprising a subject compound. A composition comprising a subject compound may further comprise a fluorescent compound or a phosphorescent compound, and may be useful for light emission in devices such as organic light-emitting devices.

[0102] In some embodiments, an organic light-emitting device comprises a subject compound. For example, an

organic component comprising a subject compound may be disposed between an anode and a cathode. The organic component may further comprise an emissive layer, wherein a subject compound is in the emissive layer. In some embodiments, the device is configured so that electrons can be transferred from the cathode to the organic component and holes can be transferred from the anode to the organic component.

[0103] The subject compounds may have high photostability and thermal stability in organic light-emitting devices. The subject compounds may also have well balanced hole and electron injection rates and mobilities. This may provide OLED devices with high efficiencies and/or long lifetimes. The subject compounds may also form amorphous solids, which may make the compounds easy to form into films.

[0104] Some embodiments may have a structure represented by FIG. 1. A hole-injection layer **10** is disposed on the anode **5**. A hole-transport layer **15** is disposed on the hole-injection layer **15**. The emissive layer **20** is disposed on the hole-transport layer **15**. An electron-transport layer **30** is disposed on the emissive layer **20**, and the cathode **35** is disposed on the electron-transport layer **30**.

[0105] The anode may be a layer comprising a conventional material such as a metal, mixed metal, alloy, metal oxide or

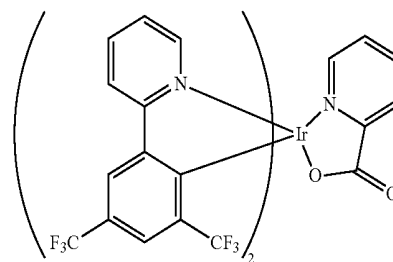
mixed-metal oxide, conductive polymer, and/or an inorganic material such as carbon nanotube (CNT). Examples of suitable metals include the Group 1 metals, the metals in Groups 4, 5, 6, and the Group 8-10 transition metals. If the anode layer is to be light-transmitting, metals in Group 10 and 11, such as Au, Pt, and Ag, or alloys thereof; or mixed-metal oxides of Group 12, 13, and 14 metals, such as indium-tin-oxide (ITO), indium-zinc-oxide (IZO), and the like, may be used. In some embodiments, the anode layer may be an organic material such as polyaniline. The use of polyaniline is described in "Flexible light-emitting diodes made from soluble conducting polymer," *Nature*, vol. 357, pp. 477-479 (11 Jun. 1992). In some embodiments, the anode layer can have a thickness in the range of about 1 nm to about 1000 nm.

[0106] A cathode may be a layer including a material having a lower work function than the anode layer. Examples of suitable materials for the cathode layer include 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 Li₂O 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 some embodiments, the cathode layer can have a thickness in the range of about 1 nm to about 1000 nm.

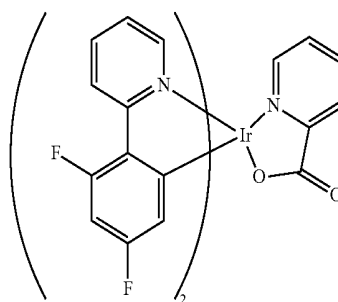
[0107] In some embodiments, the organic component may comprise at least one light-emitting layer comprising a light-emitting component and a subject compound as a host. The amount of the subject compound in a light-emitting layer may vary. In one embodiment, the amount of a subject compound in a light-emitting layer is in the range of from about 1% to about 99.9% by weight of the light-emitting layer. In another embodiment, the amount of a subject compound in a light-emitting layer is in the range of from about 90% to about 99% by weight of the light-emitting layer. In another embodiment, the amount of a subject compound in a light-emitting layer is about 97% by weight of the light-emitting layer. In some embodiments, the mass of the light-emitting component is about 0.1% to about 10%, about 1% to about 5%, or about 3% of the mass of the light-emitting layer. The light-emitting component may be a fluorescent and/or a phosphorescent compound.

[0108] A light-emitting component may comprise an iridium coordination compound such as: bis-{2-[3,5-bis(trifluoromethyl)phenyl]pyridinato-N,C2'} iridium(III)-picolinate; bis(2-[4,6-difluorophenyl]pyridinato-N,C2') iridium(III) picolinate; bis(2-[4,6-difluorophenyl]pyridinato-N,C2') iridium(acetylacetonate); Iridium(III) bis(4,6-difluorophenylpyridinato)-3-(trifluoromethyl)-5-(pyridin-2-yl)-1,2,4-triazolate; Iridium(III) bis(4,6-difluorophenylpyridinato)-5-(pyridin-2-yl)-1H-tetrazolate; bis[2-(4,6-difluorophenyl)pyridinato-N,C2'] iridium(III)tetra(1-pyrazolyl)borate; Bis[2-(2'-benzothienyl)-pyridinato-N,C3'] iridium(III) (acetylacetonate); Bis[(2-phenylquinolyl)-N,C2'] iridium(III) (acetylacetonate); Bis[(1-phenylisoquinolinato-N,C2')] iridium(III) (acetylacetonate); Bis[(dibenzo[f,h]quinoxalino-N,C2')] iridium(III) (acetylacetonate); Tris(2,5-bis-2'-(9',9'-dihexylfluorene)pyridine) iridium(III); Tris[1-phenylisoquinolinato-N,C2'] iridium(III); Tris-[2-(2'-

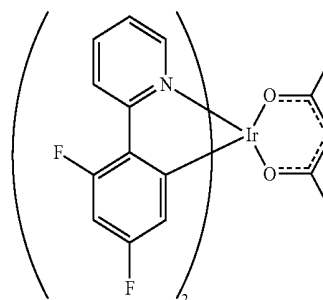
benzothienyl)-pyridinato-N,C3'] iridium(III); Tris[1-thiophen-2-ylisoquinolinato-N,C3'] iridium(III); Tris[1-(9,9-dimethyl-9H-fluoren-2-yl)isoquinolinato-(N,C3')] iridium(III); Bis(2-phenylpyridinato-N,C2') iridium(III) (acetylacetonate) [Ir(ppy)₂(acac)]; Bis(2-(4-tolyl)pyridinato-N,C2') iridium(III) (acetylacetonate) [Ir(mppy)₂(acac)]; Bis(2-(4-tert-butyl)pyridinato-N,C2') iridium(III) (acetylacetonate) [Ir(t-Buppy)₂(acac)]; Tris(2-phenylpyridinato-N,C2') iridium(III) [Ir(ppy)₃]; Bis(2-phenyloxazolinato-N,C2') iridium(III) (acetylacetonate) [Ir(op)₂(acac)]; Tris(2-(4-tolyl)pyridinato-N,C2') iridium(III) [Ir(mppy)₃]; Bis[2-phenylbenzothiazolato-N,C2'] iridium(III) (acetylacetonate); Bis[2-(4-tert-butylphenyl)benzothiazolato-N,C2'] iridium(III) (acetylacetonate); Bis[(2-(2'-thienyl)pyridinato-N,C3')] iridium(III) (acetylacetonate); Tris[2-(9,9-dimethylfluoren-2-yl)pyridinato-(N,C3')] iridium(III); Tris[2-(9,9-dimethylfluoren-2-yl)pyridinato-(N,C3')] iridium(III); Bis[5-trifluoromethyl-2-[3-(N-phenylcarzoyl)pyridinato-N,C2'] iridium(III) (acetylacetonate); (2-PhPyCz)₂Ir(III) (acac); etc.



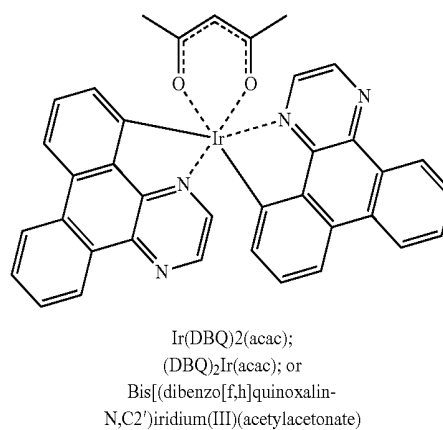
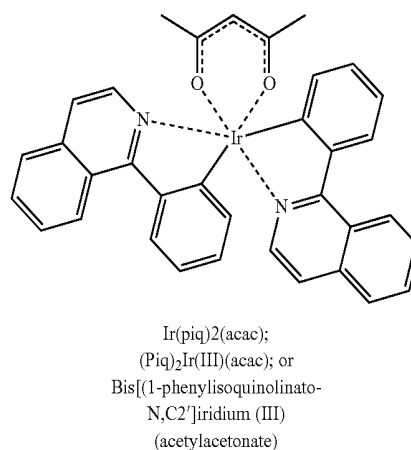
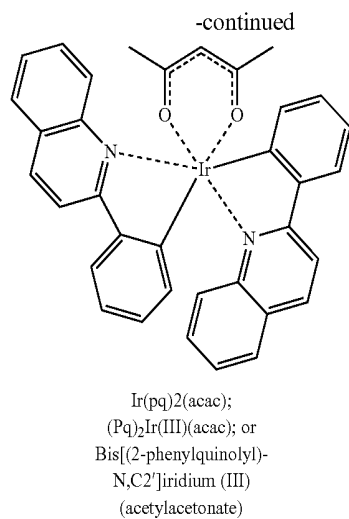
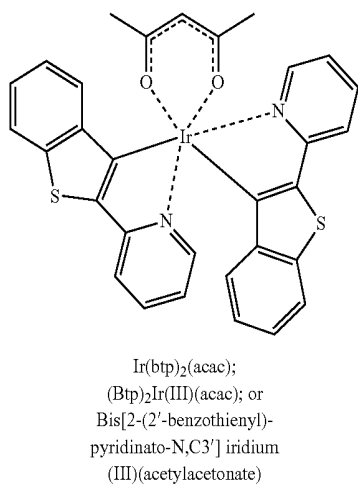
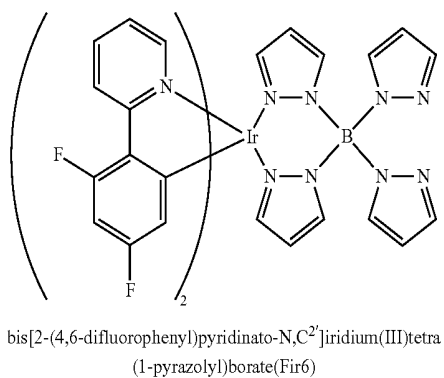
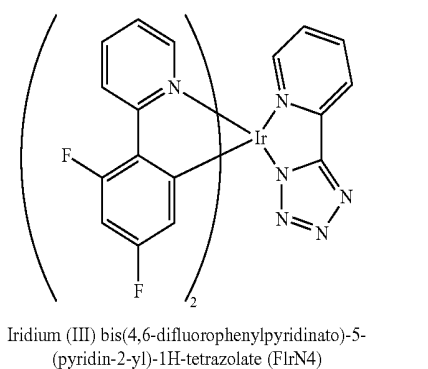
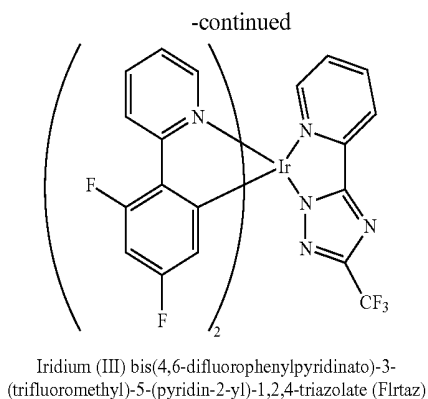
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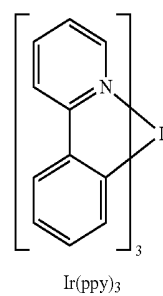
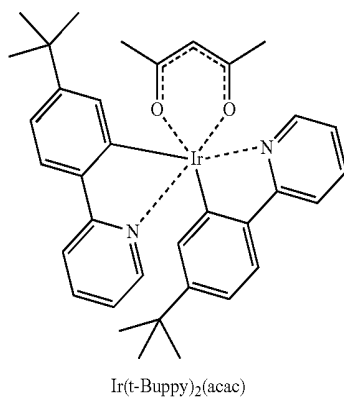
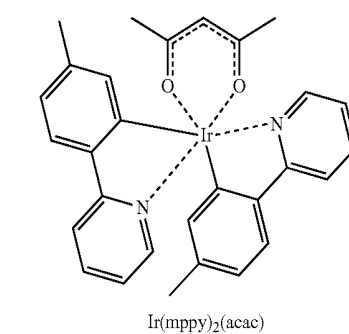
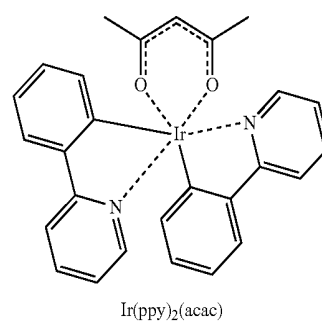
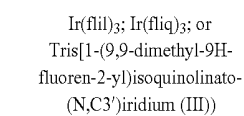
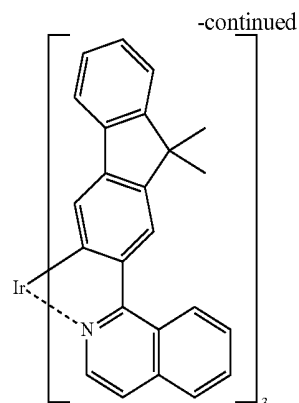
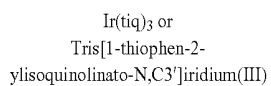
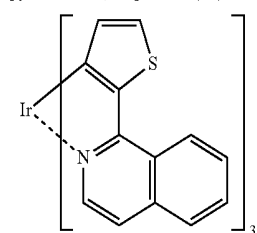
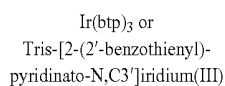
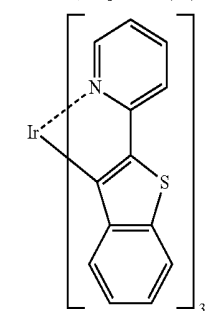
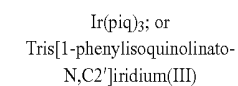
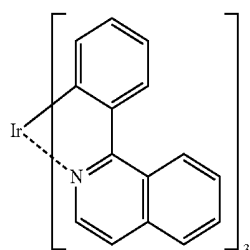
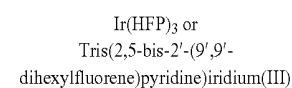
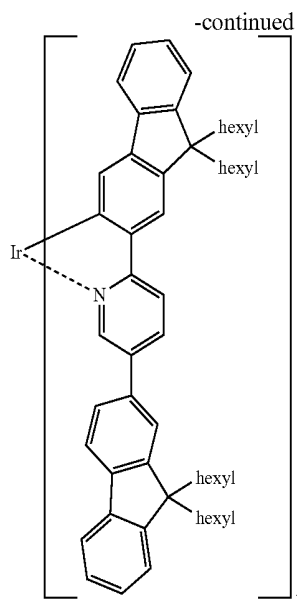


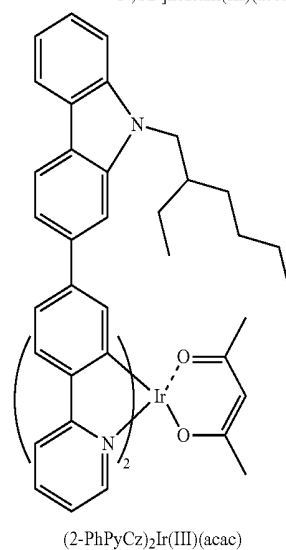
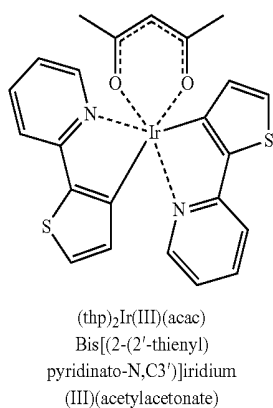
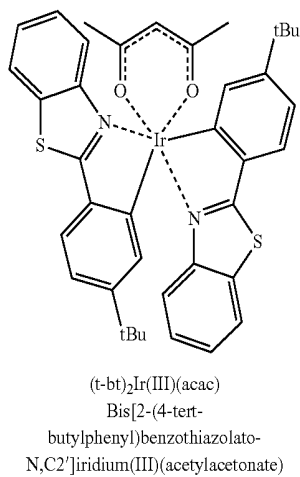
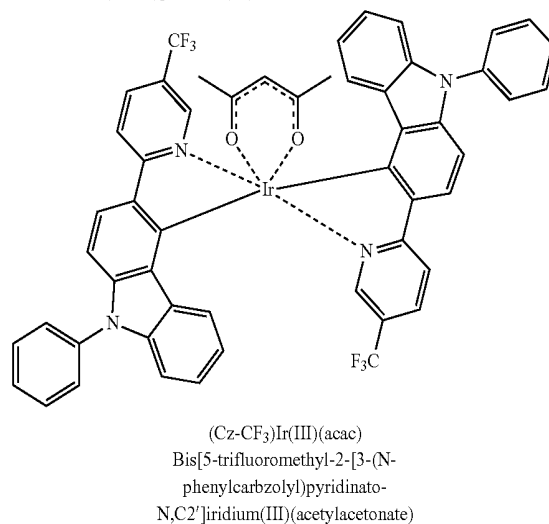
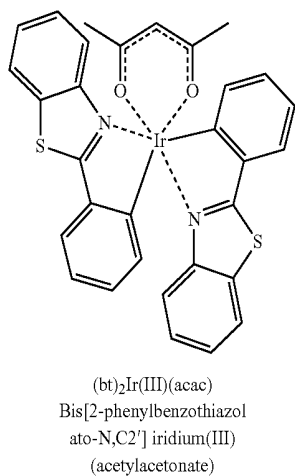
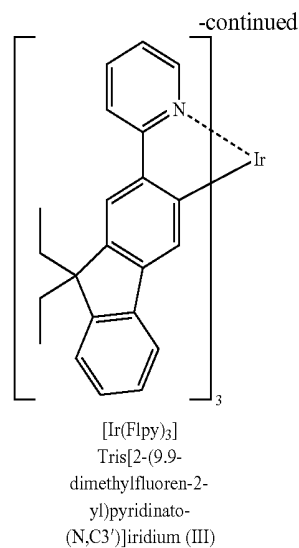
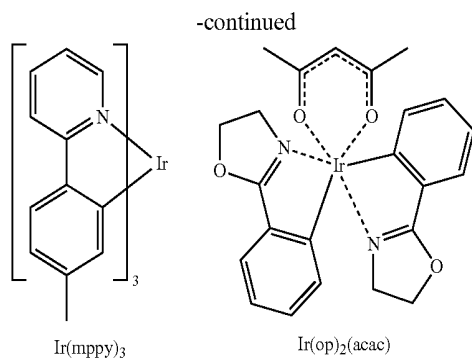
bis(2-[4,6-difluorophenyl]pyridinato-N,C2') iridium(III) picolinate [FlrPic]



bis(2-[4,6-difluorophenyl]pyridinato-N,C2') iridium(III) (acetylacetonate) [Flr(acac)]







[0109] The thickness of a light-emitting layer may vary. In one embodiment, a light-emitting layer has a thickness in the range of from about 1 nm to about 150 nm or about 200 nm.

[0110] In some embodiments, the organic component may further comprise a hole-transport layer disposed between the

anode and the light-emitting layer. The hole-transport layer may comprise at least one hole-transport material. Hole-transport materials may include, but are not limited to, an aromatic-substituted amine, a carbazole, a polyvinylcarbazole (PVK), e.g. poly(9-vinylcarbazole); polyfluorene; a polyfluorene copolymer; poly(9,9-di-n-octylfluorene-alt-benzothiadiazole); poly(paraphenylene); poly[2-(5-cyano-5-methylhexyloxy)-1,4-phenylene]; a benzidine; a phenylenediamine; a phthalocyanine metal complex; a polyacetylene; a polythiophene; a triphenylamine; an oxadiazole; copper phthalocyanine; 1,1-Bis(4-bis(4-methylphenyl)aminophenyl)cyclohexane; 2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline; 3,5-Bis(4-tert-butyl-phenyl)-4-phenyl[1,2,4]triazole; 3,4,5-Triphenyl-1,2,3-triazole; 4,4',4"-tris(3-methylphenylphenylamino)triphenylamine (MTDATA); N,N'-bis(3-methylphenyl)N,N'-diphenyl-[1,1'-biphenyl]-4,4'-diamine (TPD); 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (α -NPD); 4,4',4"-tris(carbazol-9-yl)-triphenylamine (TCTA); 4,4'-bis[N,N'-(3-tolyl)amino]-3,3'-dimethylbiphenyl (HMTDPD); 4,4'-N,N'-dicarbazole-biphenyl (CBP); 1,3-N,N-dicarbazole-benzene (mCP); Bis[4-(p,p'-ditolyl-amino)phenyl]diphenylsilane (DTASi); 2,2'-bis(4-carbazolylphenyl)-1,1'-biphenyl (4CzPBP); N,N,N"-1,3,5-tricarbazolylbenzene (tCP); N,N'-bis(4-butylphenyl)-N,N'-bis(phenyl)benzidine; or the like.

[0111] In some embodiments, the organic component may further comprise an electron-transport layer disposed between the cathode and the light-emitting layer. Examples of electron-transport materials may include, but are not limited to, 2-(4-biphenyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (PBD); 1,3-bis(N,N-t-butyl-phenyl)-1,3,4-oxadiazole (OXD-7); 1,3-bis[2-(2,2'-bipyridine-6-yl)-1,3,4-oxadiazol-5-yl]benzene; 3-phenyl-4-(1'-naphthyl)-5-phenyl-1,2,4-triazole (TAZ); 2,9-dimethyl-4,7-diphenyl-phenanthroline (bathocuproine or BCP); aluminum tris(8-hydroxyquinolate) (Alq_3); and 1,3,5-tris(2-N-phenylbenzimidazolyl)benzene; 1,3-bis[2-(2,2'-bipyridine-6-yl)-1,3,4-oxadiazol-5-yl]benzene (BPY-OXD); 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-biphenyl)-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.

[0112] If desired, additional layers may be included in the light-emitting device. These additional layers may include an electron-injecting layer (EIL), a hole-blocking layer (HBL), an exciton-blocking layer (EBL), and/or a hole-injecting layer (HIL). In addition to separate layers, some of these materials may be combined into a single layer.

[0113] In some embodiments, the light-emitting device can include an electron-injecting layer between the cathode layer and the light-emitting layer. Other suitable electron-injecting materials may also be included, and are known to those skilled in the art. Examples of suitable material(s) that can be included in the electron-injecting layer include but are not limited to, an optionally substituted compound selected from the following: aluminum quinolate (Alq_3), 2-(4-biphenyl)-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-hydroxyquinolate) aluminum, and a metal thioxinoid compound such as bis(8-quinol-

linethiolato) zinc. In one embodiment, the electron-injecting layer is aluminum quinolate (Alq_3), 2-(4-biphenyl)-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.

[0114] 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.

[0115] In some embodiments, the light-emitting device can include an exciton-blocking layer, e.g., between the light-emitting layer and the anode. In an 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.

[0116] In some embodiments, the light-emitting device can include a hole-injecting layer, e.g., between the light-emitting layer and the anode. A hole-injecting layer may comprise a subject compound as a hole-injecting material. Other examples of suitable hole-injecting material(s) include, but are not limited to, 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 triphenyl amine or phenylenediamine derivative such as N,N'-bis(4-methylphenyl)-N,N'-bis(phenyl)-1,4-phenylenediamine, 4,4',4"-tris(N-(naphthyl-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), and a phthalocyanine metal complex derivative such as phthalocyanine copper.

[0117] Light-emitting devices comprising a subject compound 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 hole-injecting and/or hole-transport layer may be deposited on the anode in that order. A light-emitting layer that includes a light-emitting component, can be deposited on the anode, the hole-transport layer, or the hole-injecting layer. The light-emitting layer may contain a subject compound. An electron-transport layer and/or an electron-injecting layer may be deposited in that order on the light-emitting component. The cathode layer, comprising a low work functioning metal (e.g., Mg:Ag), can then be deposited, e.g., by vapor deposition or sputtering. The device may also con-

tain an exciton-blocking layer, an electron blocking layer, a hole blocking layer, a second light-emitting layer, or other layers that can be added to the device using suitable techniques.

[0118] In some embodiments, a device comprising the subject compounds can provide a significantly increased device lifetime compared with commercially available compounds. In some embodiments, the devices can provide a T50(h) @ 10000 nit lifetime of at least about 125, 150, 175, 185, and/or 200 hours. In some embodiments, the desired lifetime can be determined by examining the luminescent/emissive decay of the device by measuring the luminescent, e.g., cd/m², after applying a constant current of a 16 mA to device (corresponding to about 10000 cd/m²) for a device having an active emissive area of about 13.2 mm².

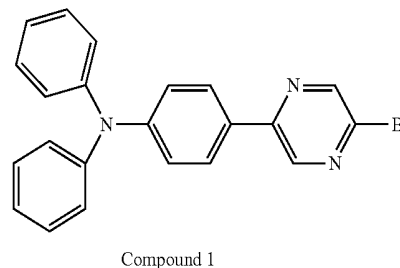
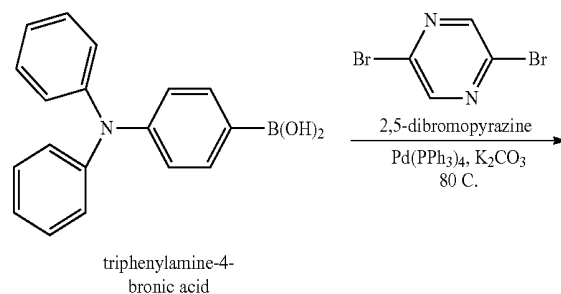
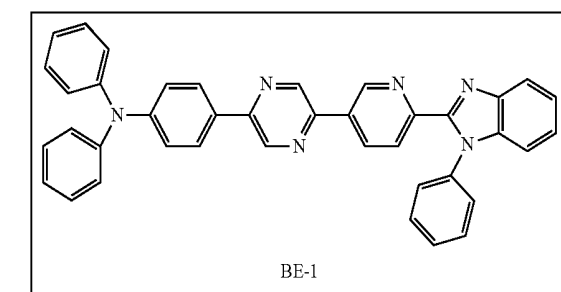
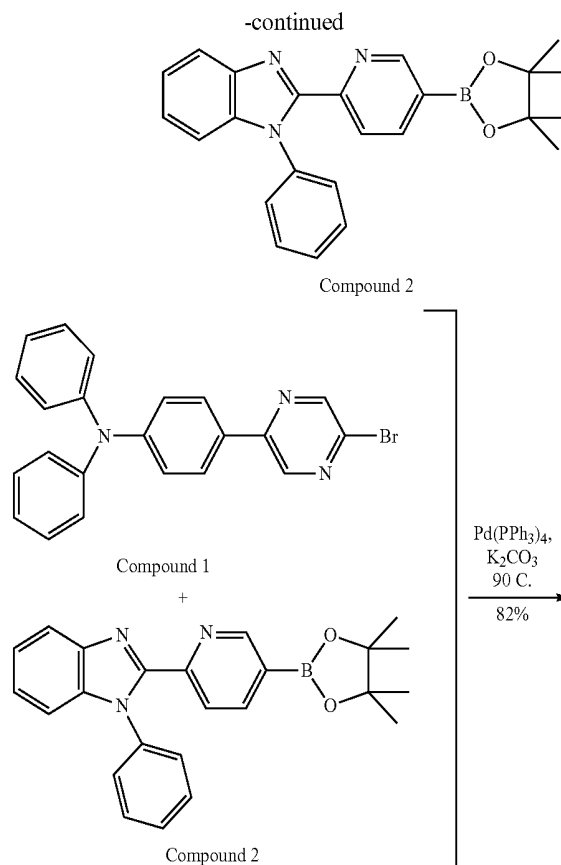
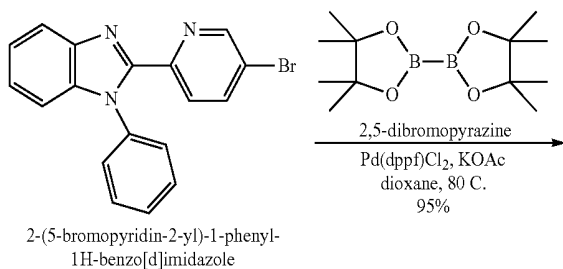
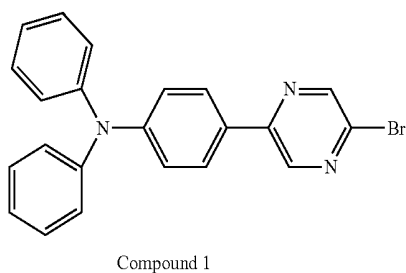
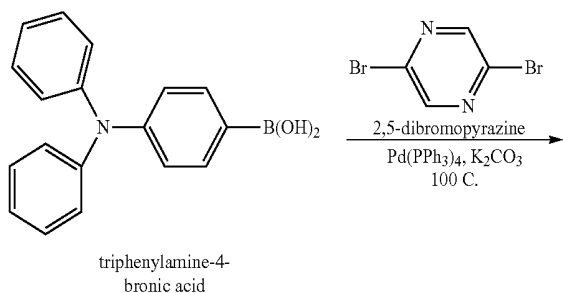
3. Synthetic Examples

4. Example 1.1

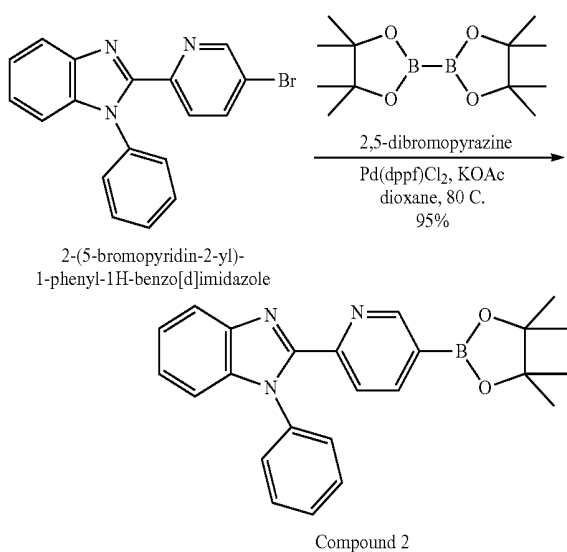
8-1. Example of Synthesis

Synthesis of BE-1

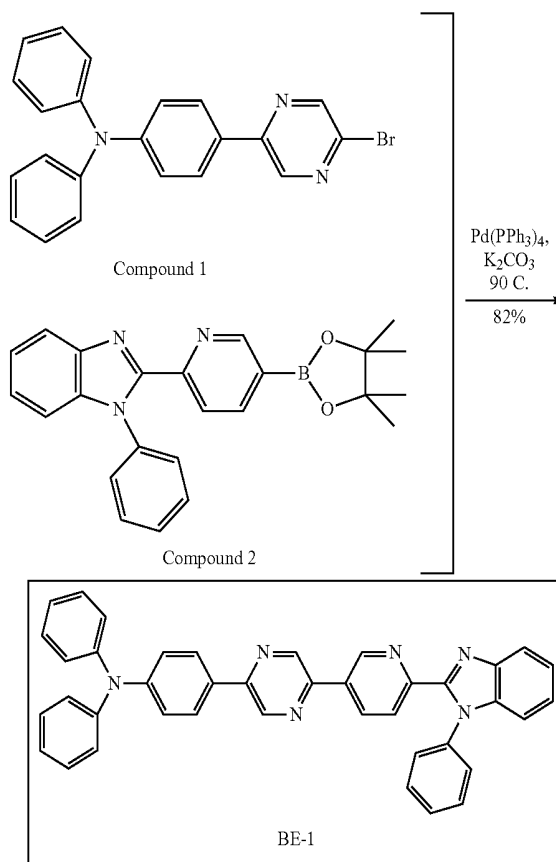
[0119]



[0120] 4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline (Compound 1): A mixture of triphenylamine-4-bromic acid (1.0 g, 3.46 mmol), 2,5-dibromopyrazine (1.81 g, 7.6 mmol), Pd(PPh₃)₄ (0.2 g, 0.17 mmol) and K₂CO₃ (1.05 g, 7.6 mmol) in dioxane/water (40 mL/8 mL) was degassed and heated at about 80° C. for about 15 hours. The whole was worked up with ethyl acetate (200 mL), washed with brine. The organic phase was dried over Na₂SO₄, loaded on silica gel, purified by flash column using the eluents of hexanes to hexanes/dichloromethane (2:1 to 1:1 to 1:2). The desired fraction was collected, and removal of solvent gave a yellow solid (Compound 1) (0.99 g, in 71% yield).



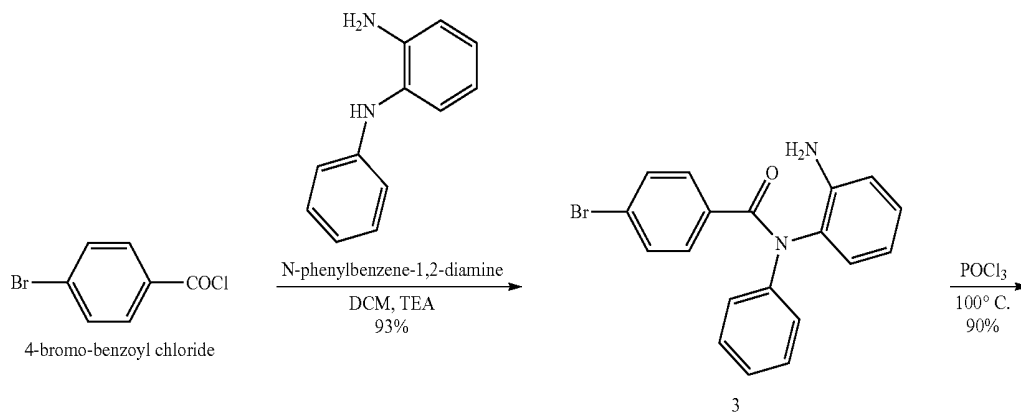
[0121] 1-Phenyl-2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)-1H-benzodimidazole (Compound 2): A mixture of 2-(5-bromopyridin-2-yl)-1-phenyl-1H-benzodimidazole (1.015 g, 2.9 mmol), bis(pinacolato)diboron (0.76 g, 3 mmol), KOAc (0.49 g, 5 mmol) and Pd(dppf)Cl₂ (0.11 g, 0.15 mmol) in dioxane (50 mL) was degassed and heated at about 80° C. for about 15 hours. The whole was worked up with dichloromethane/brine. The organic phase was collected and dried over Na₂SO₄. After removal of solvent, the resulting brown oil (Compound 2) was used for next step without further purification.



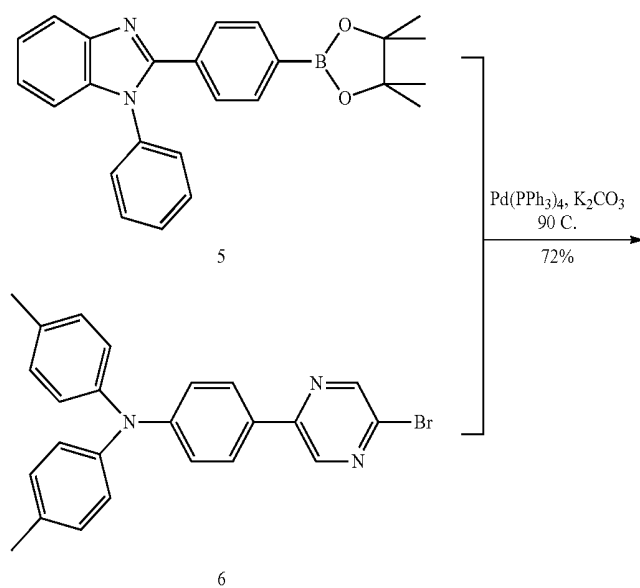
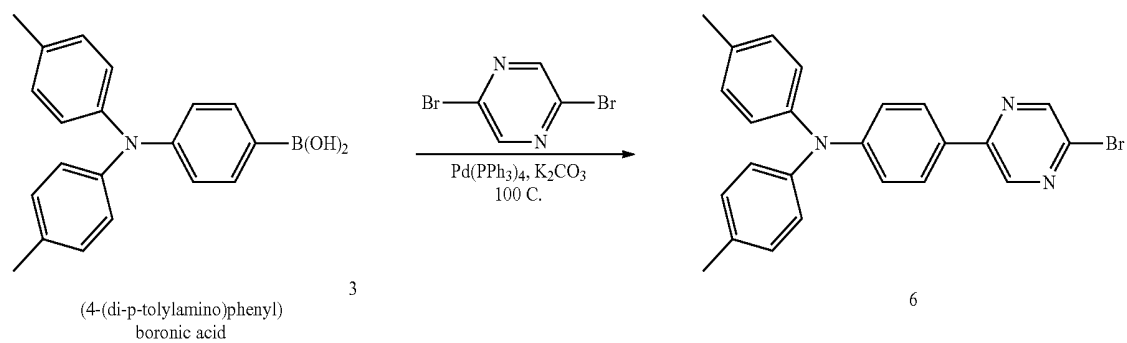
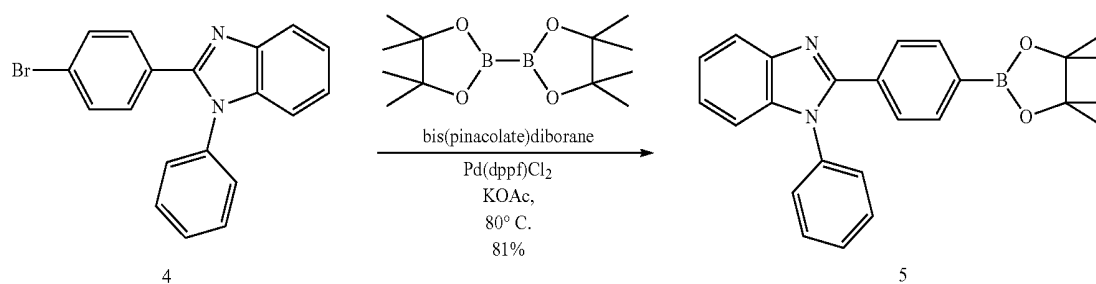
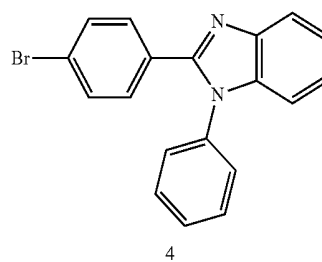
[0122] Compound BE-1: A mixture of 4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline (Compound 1) (0.99 g, 2.46 mmol), 1-phenyl-2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)-1H-benzodimidazole (Compound 2) (1.15 g, 2.9 mmol), Pd(PPh₃)₄ (0.22 g, 0.19 mmol) and K₂CO₃ (1.0 g, 7.2 mmol) in dioxane/water (60 mL/10 mL), was degassed and heated at about 85° C. overnight. Yellow precipitate formed. After filtration, the solid was collected and washed with methanol, then hot dichloromethane (500 mL). A yellow solid (BE-1) was collected, 1.20 g, in 82% yield. Confirmed by LCMS (APCI+): calcd for C₄₀H₂₉N₆ (M+H): 593; found 593.

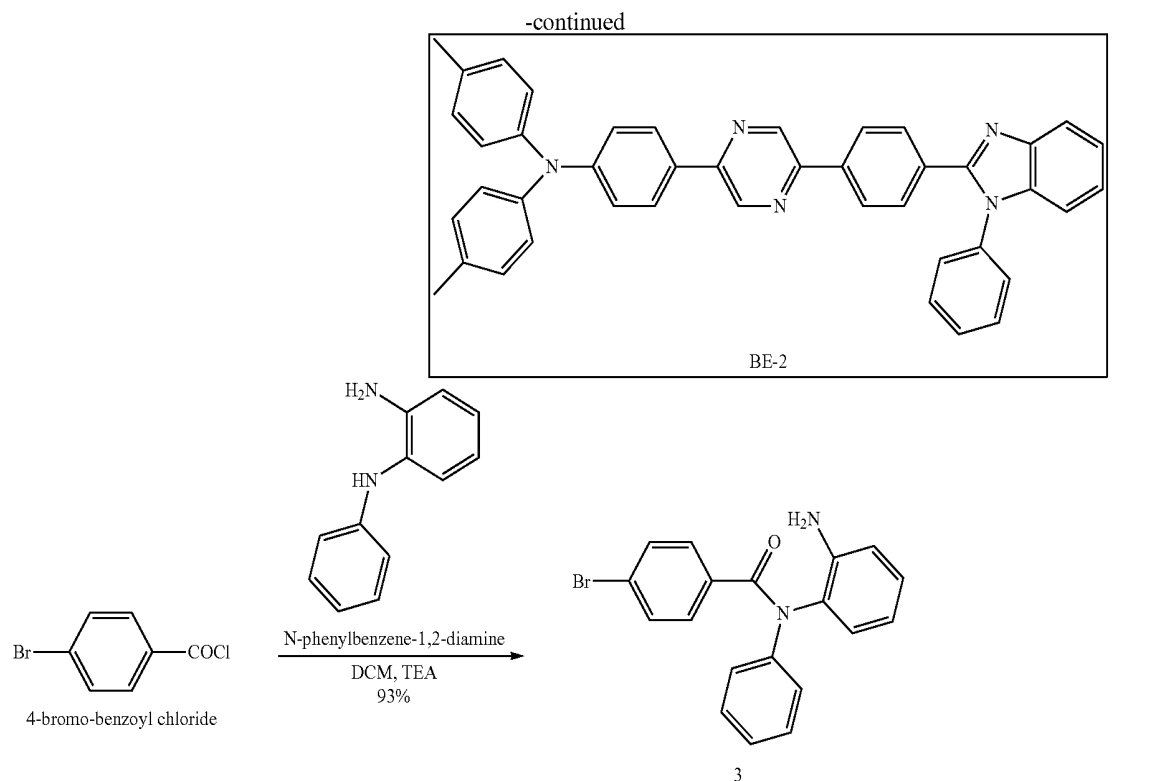
Synthesis of BE-2

[0123]



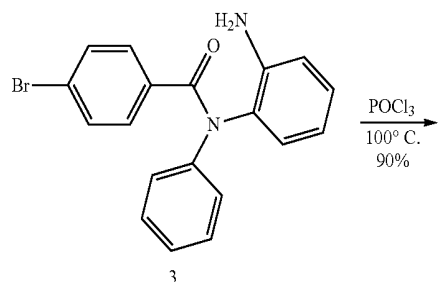
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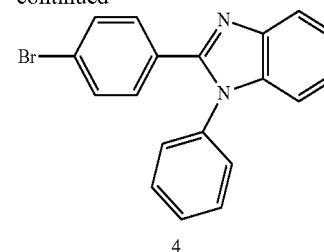


4-Bromo-N-(2-(phenylamino)phenyl)benzamide
(Compound 3)

[0124] To a solution of 4-bromo-benzoyl chloride (11 g, 50 mmol) in anhydrous dichloromethane (DCM) (100 ml), was added N-phenylbenzene-1,2-diamine (10.2 g, 55 mmol), then triethylamine (TEA) (17 ml, 122 mmol) slowly. The whole was stirred at room temperature (RT) overnight. Filtration gave a white solid 3 (6.5 g). The filtrate was worked up with water (300 ml), then extracted with DCM (300 mL) three times. The organic phase was collected and dried over MgSO_4 , concentrated and recrystallized in DCM/hexanes to give another portion of white solid 3 (10.6 g). Total amount of product 3 is 17.1 g, in 93% yield.

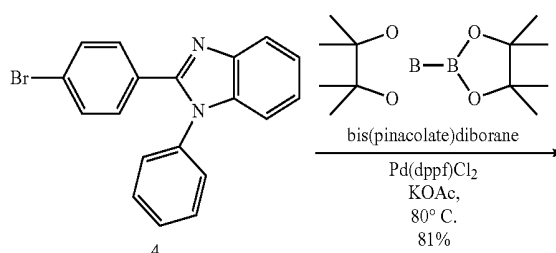


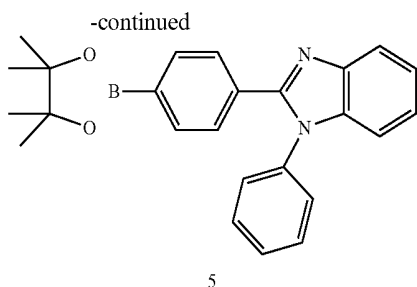
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2-(4-bromophenyl)-1-phenyl-1H-benzo[d]imidazole
(4)

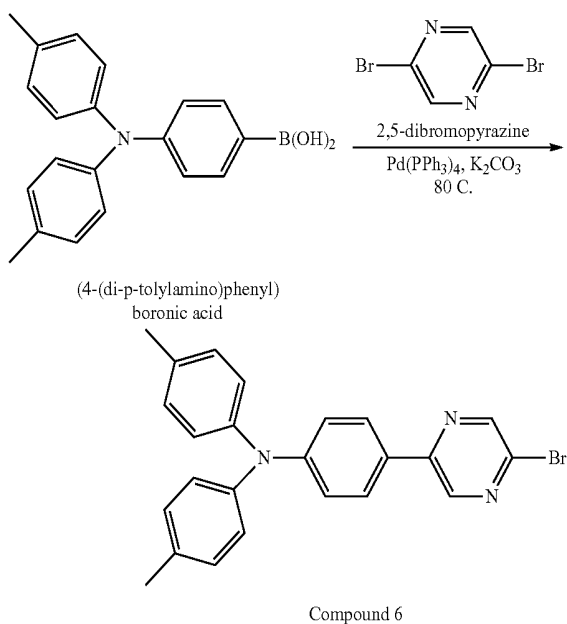
[0125] To a suspension of amide 3 (9.6 g, 26 mmol) in anhydrous 1,4-dioxane (100 mL) was added phosphorus oxychloride (POCl_3) (9.2 mL, 100 mmol) slowly. The whole was then heated at 100°C. overnight. After cooling to RT, the mixture was poured into ice (200 g) with stirring. Filtration, followed by recrystallization in DCM/hexanes gave a pale grey solid 4 (8.2 g, in 90% yield).





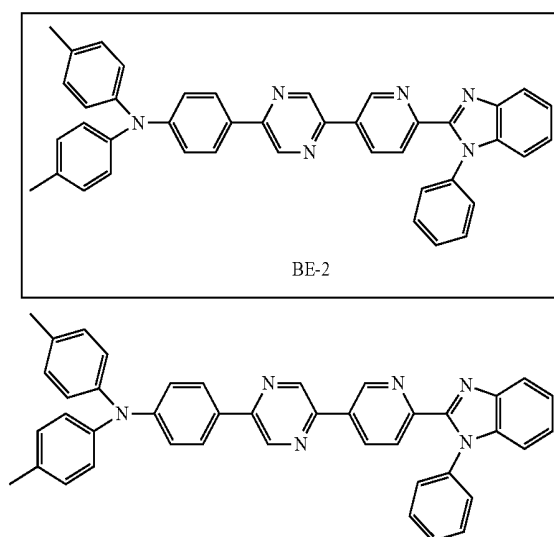
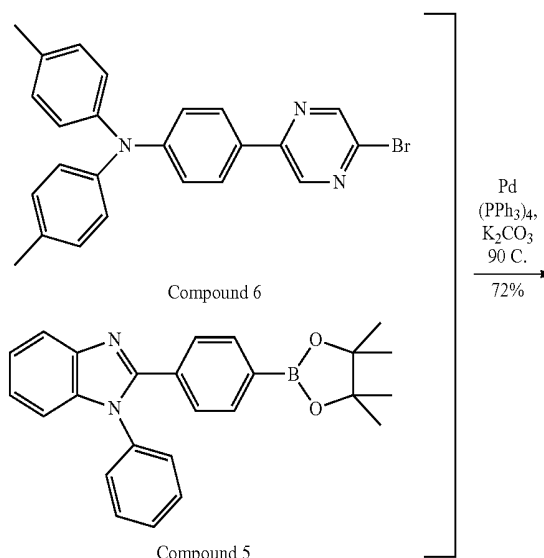
1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzimidazole (5)

[0126] A mixture of Compound 4 (0.70 g, 2 mmol), bis(pinacolate)diborane (0.533 g, 2.1 mmol), bis(diphenylphosphino)ferrocene]dichloropalladium ($\text{Pd}(\text{dppf})\text{Cl}_2$) (0.060 g, 0.08 mmol) and anhydrous potassium acetate (KOAc) (0.393 g, 4 mmol) in 1,4-dioxane (20 ml) was heated at about 80° C. under argon overnight. After cooling to RT, the whole was diluted with ethyl acetate (80 ml) then filtered. The solution was absorbed on silica gel, then purified by column chromatography (hexanes/ethyl acetate 5:1 to 3:1) to give a white solid 5 (0.64 g, in 81% yield).



4-(5-bromopyrazin-2-yl)-N,N-di-p-tolylaniline (Compound 6)

[0127] A mixture of (4-(di-p-tolylamino)phenyl)boronic acid (0.74 g, 2.33 mmol), 2,5-dibromopyrazine (1.19 g, 5 mmol), $\text{Pd}(\text{PPh}_3)_4$ (0.14 g, 0.12 mmol) and K_2CO_3 (0.69 g, 5 mmol) in dioxane/water (80 mL/10 mL) was degassed and heated at about 80° C. overnight. The whole was diluted with ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4 , loaded on silica gel column and purified by flash column using eluents of hexanes to hexanes/dichloromethane (3:1). The desired fraction was collected, and a yellow solid (6) was obtained after removal of solvents, 0.63 g, in 63% yield.

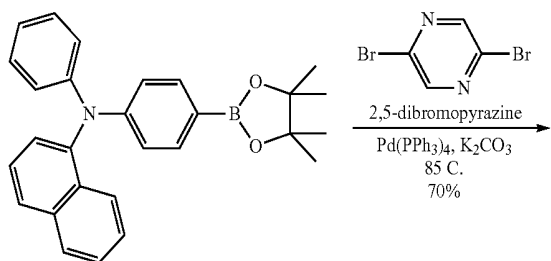


Chemical Formula: $\text{C}_{43}\text{H}_{33}\text{N}_5$
Molecular Weight: 619.76

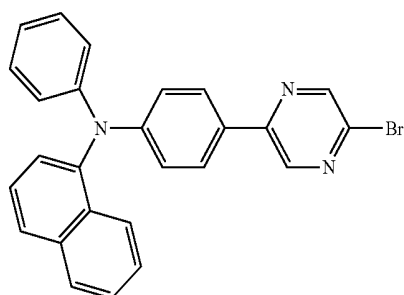
Compound BE-2

[0128] A mixture of 4-(5-bromopyrazin-2-yl)-N,N-di-p-tolylaniline (Compound 6) (0.63 g, 1.46 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzimidazole (Compound 5) (0.58 g, 1.46 mmol), $\text{Pd}(\text{PPh}_3)_4$ (0.115 g, 0.1 mmol) and K_2CO_3 (0.414 g, 3 mmol) in dioxane/water (50 mL/10 mL) was degassed and heated at about 90° C. overnight. The resulting solution was diluted with ethyl acetate (250 mL), washed with brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes to dichloromethane to dichloromethane/ethyl acetate 4:1. The desired yellow fraction was collected, concentrated, recrystallized in dichloromethane/hexanes to give a yellow crystalline solid (Compound 6) (0.74 g, in 82% yield). Confirmed by LCMS (APCI+): calcd for $\text{C}_{43}\text{H}_{34}\text{N}_5$ (M+H): 620; found: 620.

loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane (8:1 to 6:1 to 2:1). The desired fraction was collected, and after removal of solvent to give a white solid (Compound 7) (6.0 g, in 75% yield).



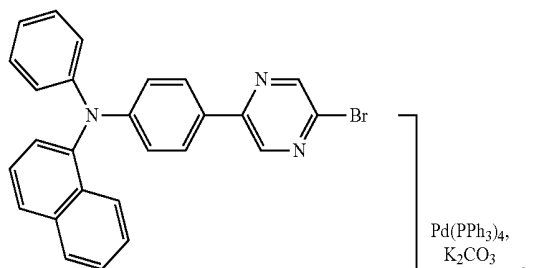
Compound 7



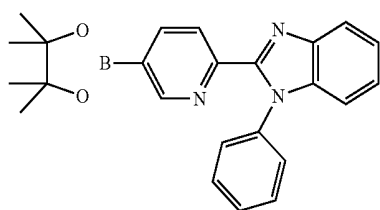
Compound 8

N-(4-(5-bromopyrazin-2-yl)phenyl)-N-phenylnaphthalen-1-amine (Compound 8)

[0131] A mixture of N-phenyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)naphthalen-1-amine (Compound 7) (2.91 g, 6.91 mmol), 2,5-dibromopyrazine (3.56 g, 13.8 mmol), Pd(PPh₃)₄ (0.346 g, 0.3 mmol), K₂CO₃ (1.93 g, 14 mmol) in dioxane/water (80 mL/15 mL), was degassed and heated at about 85° C. overnight. The resulting mixture was diluted with ethyl acetate (250 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1 to 2:1 to 3:2). The desired fraction was collected, after removal of solvent to give a yellow solid (Compound 8) (2.2 g, in 70.4% yield).

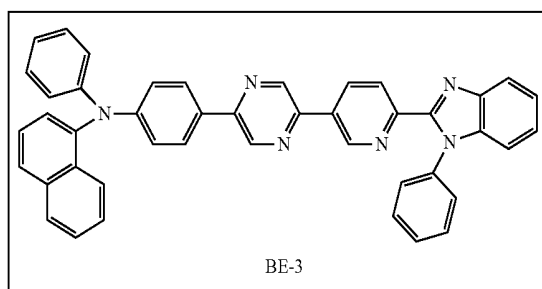


Compound 8



Compound 2

-continued

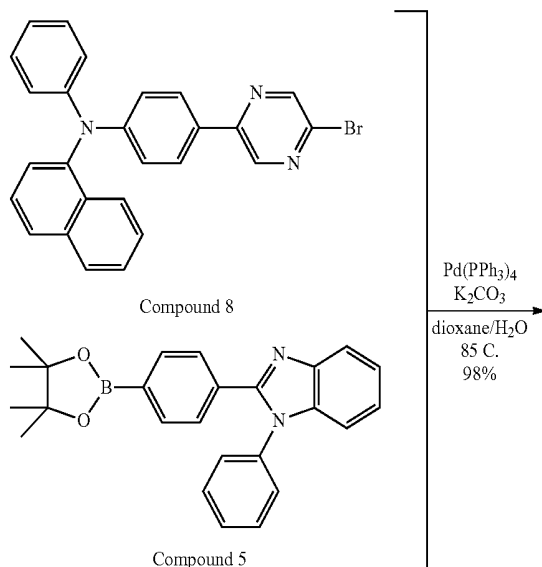


BE-3

Compound BE-3

[0132] a mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-phenylnaphthalen-1-amine (Compound 8) (1.17 g, 2.6 mmol), 1-phenyl-2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)-1H-benzo[d]imidazole (Compound 2) (2.9 mmol), Pd(PPh₃)₄ (0.138 g, 0.12 mmol) and K₂CO₃ (0.69 g, 5 mmol) in dioxane/water (70 mL/16 mL) was degassed and heated at about 90° C. overnight. The resulting mixture was diluted with ethyl acetate (200 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes/dichloromethane 1:1 to 1:2 to dichloromethane to dichloromethane/ethyl acetate 10:1 to 4:1. The desired fraction was collected and concentrated to give a yellow solid (1.39 g, in 83% yield). Confirmed by LCMS (APCI+): calcd for C₄₄H₃₁N₆ (M+H): 643; found: 643.

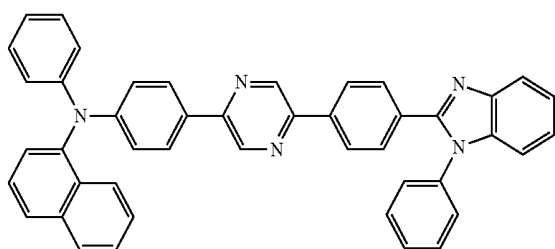
Synthesis of BE-4



Compound 8

Compound 5

-continued

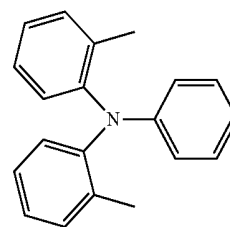
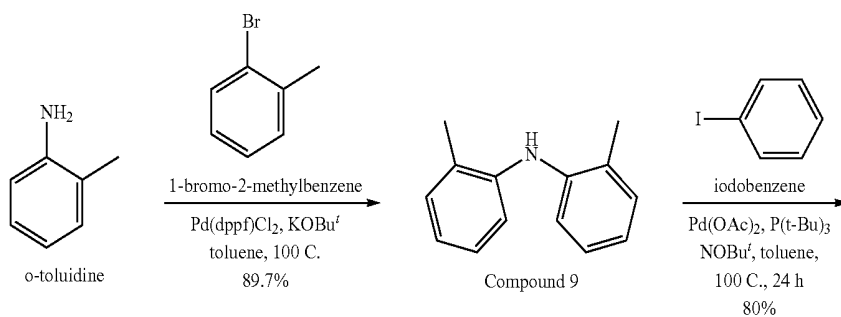


BE-4

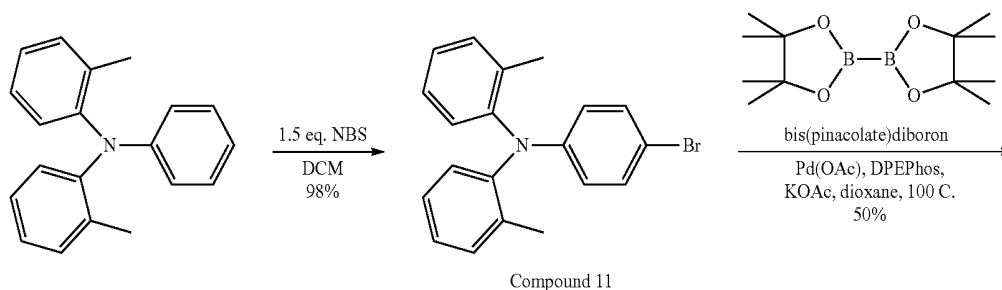
Compound BE-4

[0133] A mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-phenyl-1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (Compound 5) (0.95 g, 2.4 mmol), Pd(PPh₃)₄ (0.14 g, 0.12 mmol) and K₂CO₃ (0.69 g, 5 mmol) in dioxane/water (70 mL/15 mL) was degassed and heated at 85° C. overnight. The mixture was diluted with ethyl acetate (200 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes/dichloromethane 1:1 to dichloromethane to dichloromethane/ethyl acetate 9:1. The desired fraction was collected, concentrated and recrystallized in dichloromethane/hexanes to give yellow solid (BE-4) (1.50 g, in 98% yield). Confirmed by LCMS (APCI+): calcd for C₄₅H₃₂N₅ (M+H): 642; Found: 642.

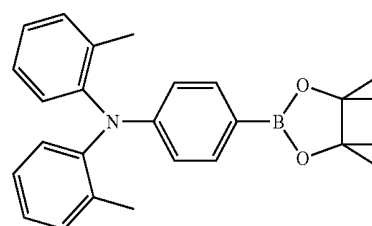
Synthesis of BE-5



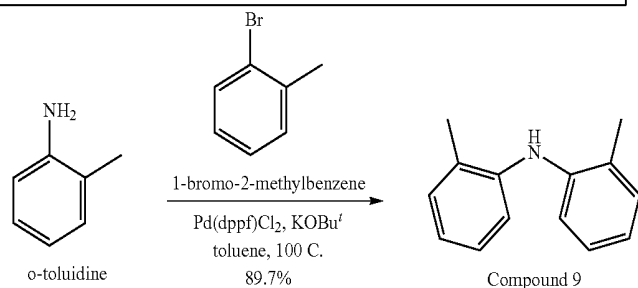
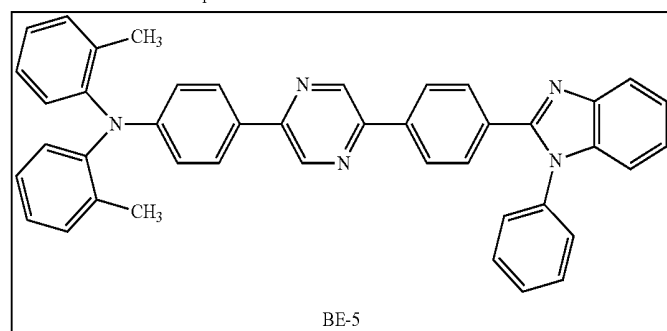
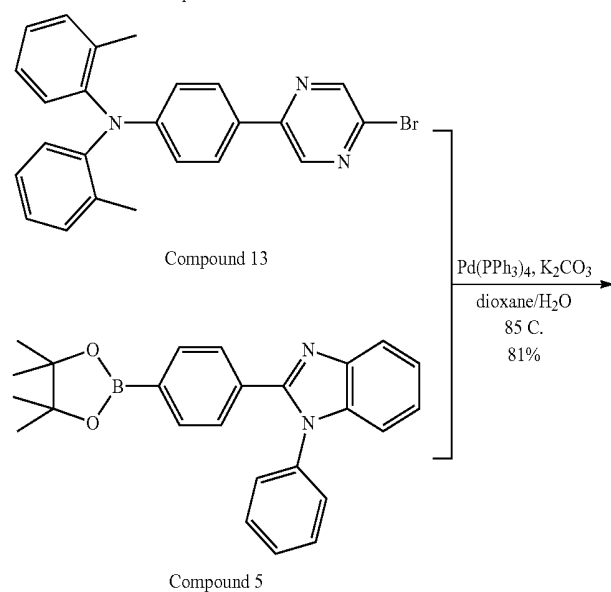
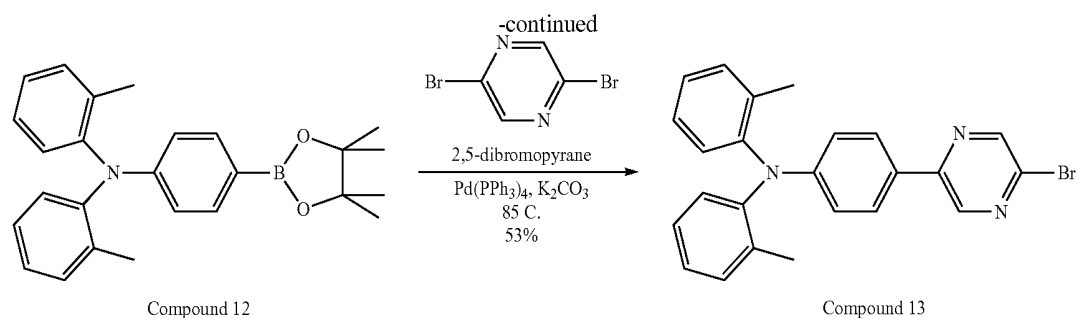
Compound 10



Compound 11

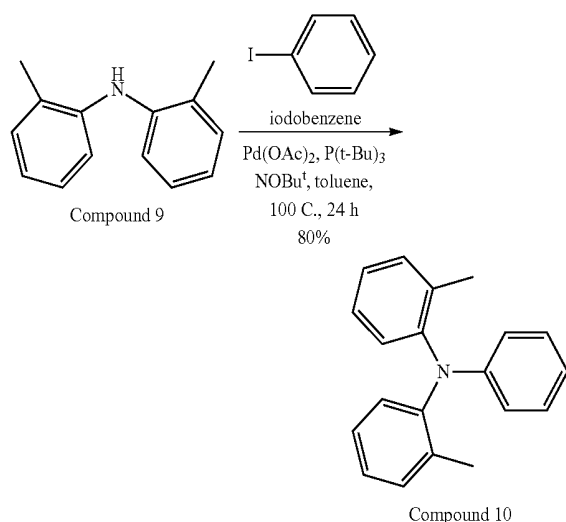


Compound 12



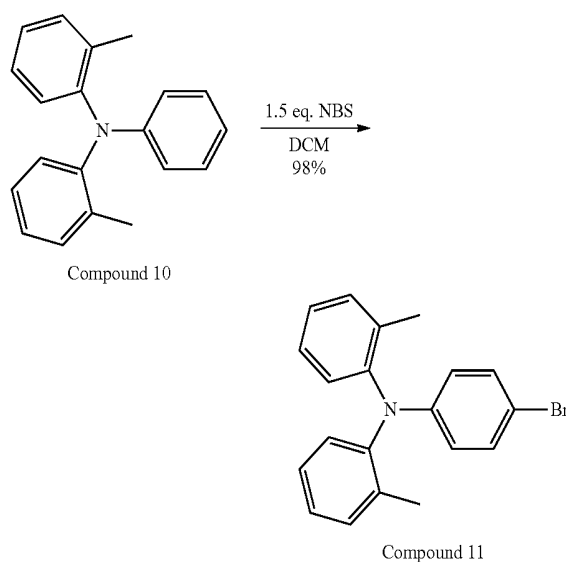
di-o-tolylamine (Compound 9)

[0134] A mixture of o-toluidine (6.05 g, 56.5 mmol), 1-bromo-2-methylbenzene (8.5 g, 50 mmol), Pd(dppf)Cl₂ and sodium tert-butoxide (9.6 g, 0.1 mmol) in toluene (120 mL) was degassed and heated at about 100° C. overnight. The mixture was purified by flash column using eluents of hexanes/dichloromethane 2:1 to give a white solid (Compound 9) (8.84 g, in 89.7% yield).



2-methyl-N-phenyl-N-(o-tolyl)aniline (Compound 10)

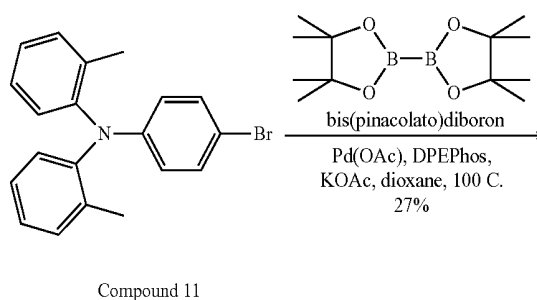
[0135] A mixture of di-o-tolylamine (Compound 9) (6.00 g, 30.4 mmol), iodobenzene (12.2 g, 60 mmol), $\text{Pd}(\text{OAc})_2$ (0.34 g, 1.5 mmol), $\text{P}(\text{t-Bu})_3$ (0.6 g, 3 mmol), sodium tert-butoxide (5.76 g, 60 mmol) in toluene (120 mL) was degassed and heated at about 120° C. for 40 hours. The resulting mixture was diluted with ethyl acetate (200 mL), washed with brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes to give a white solid (Compound 10) (8.2 g, in 98% yield).



N-(4-bromophenyl)-2-methyl-N-(o-tolyl)aniline (Compound 11)

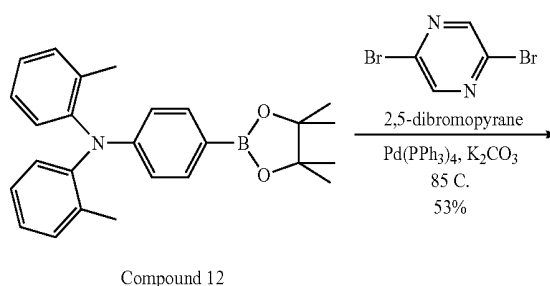
[0136] To a solution of 2-methyl-N-phenyl-N-(o-tolyl)aniline (Compound 10) (8.2 g, 30 mmol) in dichloromethane (DCM) (100 mL), was added n-bromosuccinimide (NBS) (5.34 g, 30 mmol) at about 0° C. and stirred for about 4 hours.

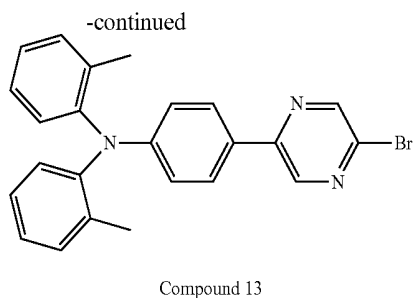
The resulting mixture was worked up with dichloromethane/brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. The desired fraction was collected, and removal of solvent gave a white solid (Compound 11) (10.7 g, in 100% yield).



2-methyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)aniline (Compound 12)

[0137] A mixture of N-(4-bromophenyl)-2-methyl-N-(o-tolyl)aniline (Compound 11) (10.7 g, 30.4 mmol), bis(pinacolato)diboron (10.16 g, 40 mmol), KOAc (6.0 g, 0.1 mol), $\text{Pd}(\text{OAc})_2$ (0.336 g, 1.5 mmol), Bis(2-diphenylphosphino)ether (1.614 g, 3 mmol) in dioxane (100 mL) was degassed and heated at about 100° C. overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1. The desired fraction was collected and the solvent was removed to give a colorless oil (Compound 12) (3.3 g, in 27% yield).



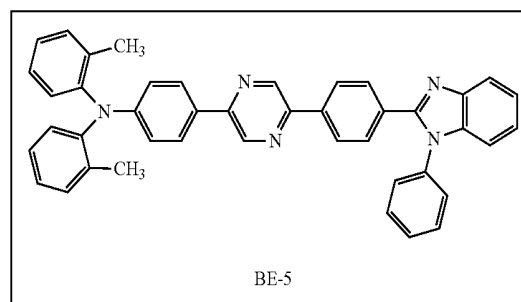


N-(4-(5-bromopyrazin-2-yl)phenyl)-2-methyl-N-(o-tolyl)aniline (Compound 13)

[0138] 2-methyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)aniline (Compound 12) (3.3 g, 8.3 mmol), 2,5-dibromopyrazine (4.27 g, 16 mmol), Pd(PPh₃)₄ (0.46 g, 0.4 mmol), K₂CO₃ (2.21 g, 16 mmol) in dioxane/water (100 mL/16 mL), was degassed and heated at about 80° C. overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na₂SO₄, loaded on silica gel, purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1 to 6:1 to 4:1). The desired fraction was collected, and a yellow solid (Compound 13) was obtained after removal of solvents (1.9 g, in 53% yield).



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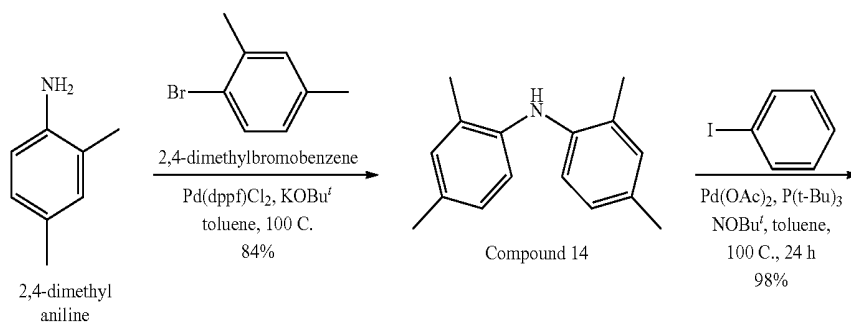


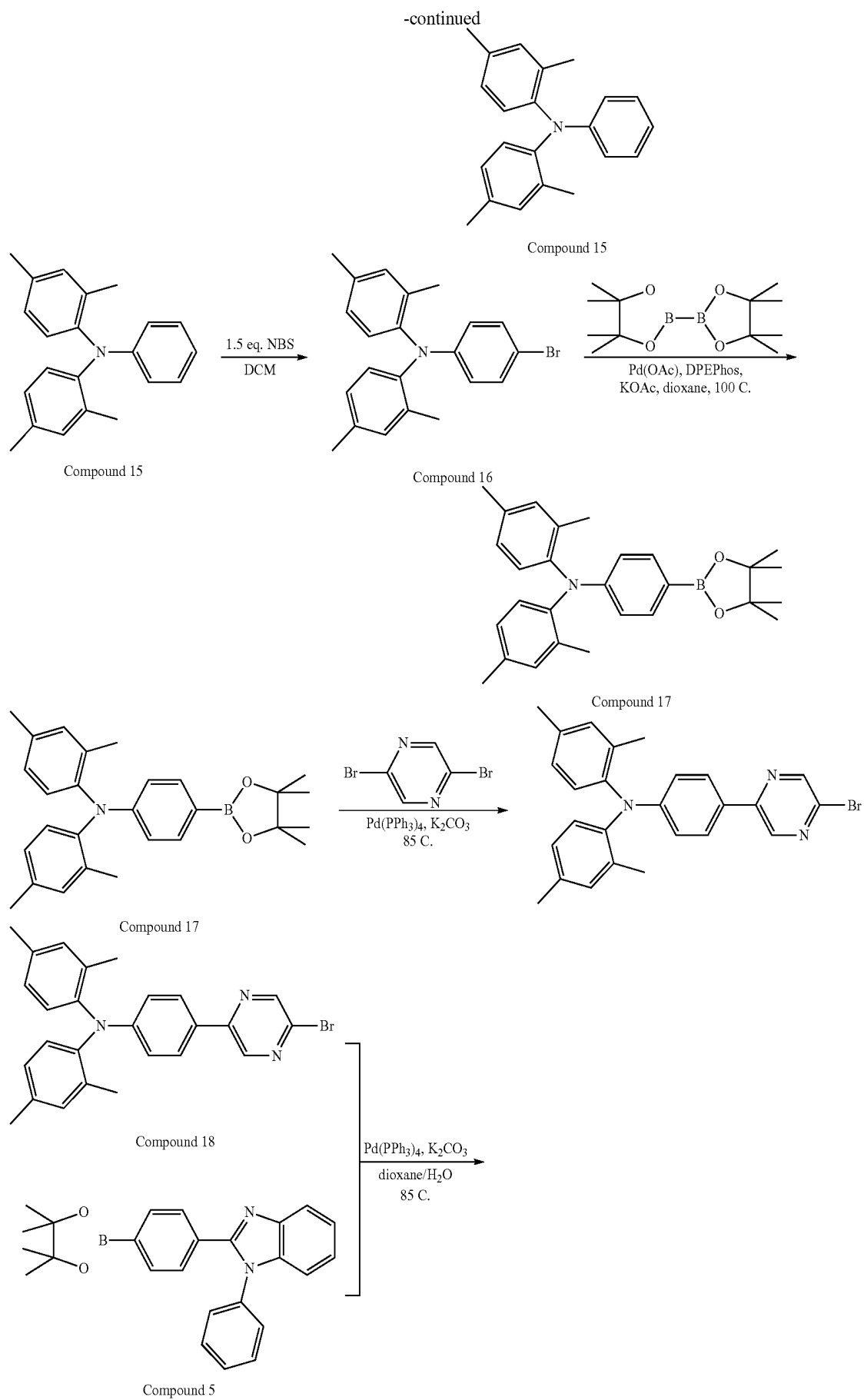
Compound BE-5

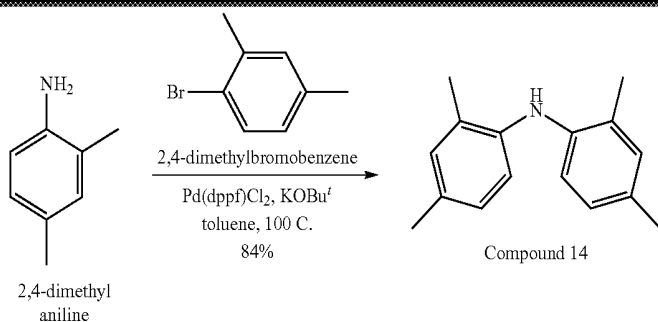
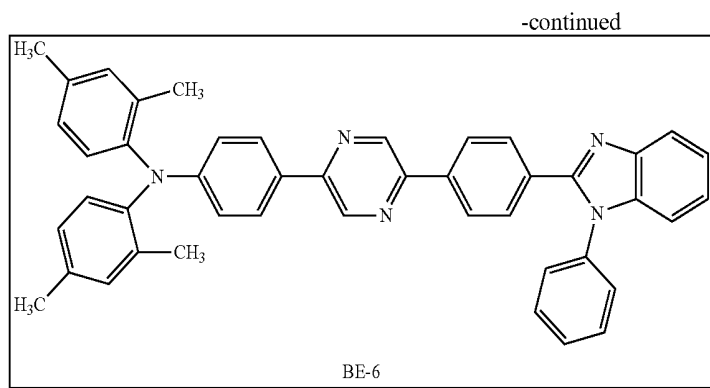
[0139] a mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-2-methyl-N-(o-tolyl)aniline (Compound 13) (1.9 g, 4.4 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (Compound 5) (1.75 g, 4.4 mmol), Pd(PPh₃)₄ (0.25 g, 0.22 mmol), K₂CO₃ (1.38 g, 10 mmol) in dioxane/water (100 mL/16 mL), was degassed and heated at about 90° C. overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 8:1 to 4:1 to dichloromethane/ethyl acetate 9:1. The desired fraction was collected, and after removal of solvent and recrystallization, gave a yellow solid (Compound BE-5) (2.2 g, in 80.6% yield). Confirmed by LCMS (APCI+): calcd for C₄₃H₃₄N₅ (M+H): 620; found: 620.

Synthesis of BE-6

[0140]



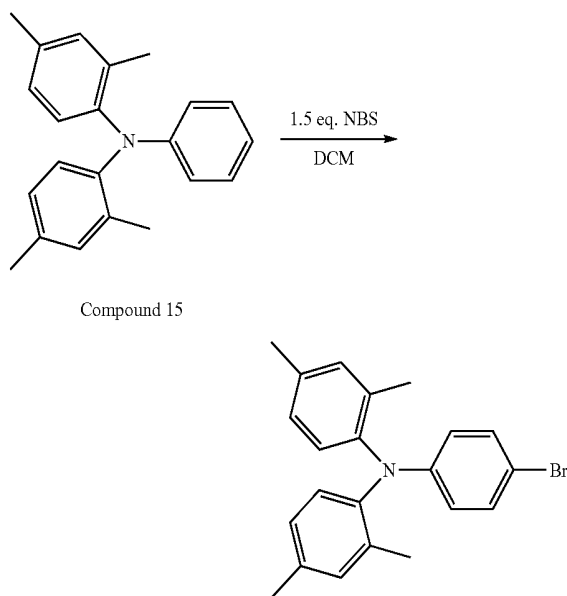
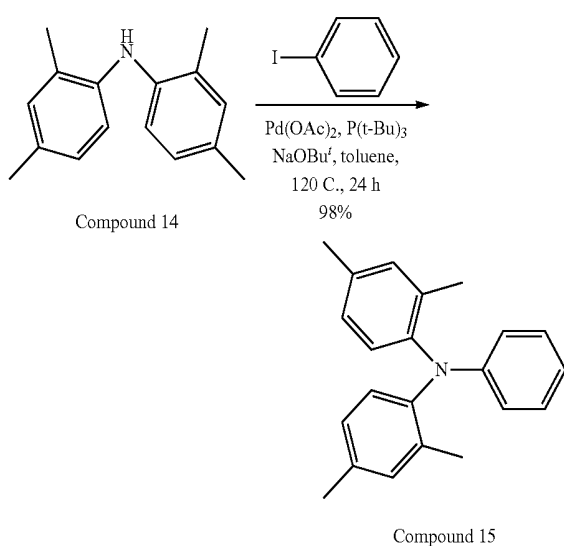




Bis(2,4-dimethylphenyl)amine (Compound 14)

[0141] A mixture of 2,4-dimethylaniline (6.05 g, 50 mmol), 2,4-dimethylbromobenzene (9.25 g, 50 mmol), Pd(dppf)Cl₂ (0.88 g, 1.2 mmol), sodium tert-butoxide (KOBU^t) (9.6 g, 0.1 mmol) in toluene (120 mL) was degassed and heated at 100° C. overnight. The resulting mixture was worked up with dichloromethane/brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. After removal of solvent, a liquid was obtained (9.45 g, in 84% yield).

mmol), Pd(OAc)₂ (0.47 g, 2.1 mmol), P(t-Bu)₃ (0.848 g, 4.2 mmol), sodium tert-butoxide (7.68 g, 80 mmol) in toluene (120 mL) was degassed and heated at 120° C. for 16 hours. The resulting mixture was poured into ethyl acetate (250 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluent of hexanes. After removal of solvent, an oil (Compound 15) was obtained (12.4 g, in 98.6% yield).

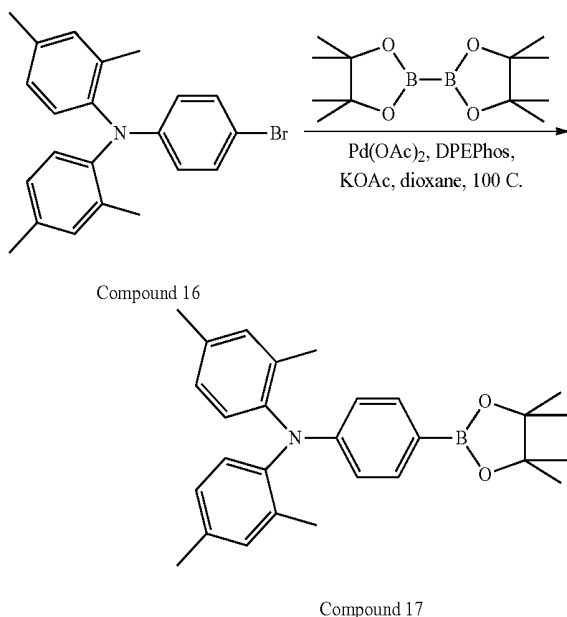


N-(2,4-dimethylphenyl)-2,4-dimethyl-N-phenylaniline (Compound 15)

[0142] A mixture of bis(2,4-dimethylphenyl)amine (Compound 14) (9.4 g, 41.8 mmol), iodobenzene (17.14 g, 84

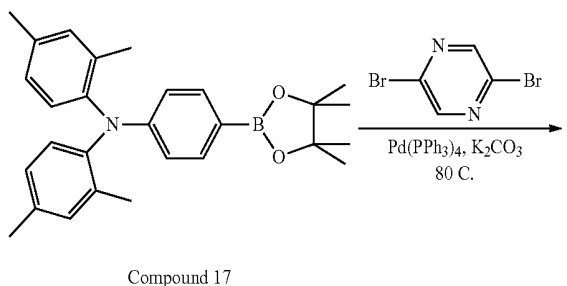
N-(4-bromophenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (Compound 16)

[0143] To a solution of N-(2,4-dimethylphenyl)-2,4-dimethyl-N-phenylaniline (Compound 15) (12.4 g, 41 mmol) in dichloromethane (200 mL), was added NBS (8.01 g, 45 mmol) at 0° C. The whole was stirred for about 3 hours and worked up with brine. The organic phase was dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes. After removal of solvents, a colorless oil (Compound 16) was obtained (15 g, in 96% yield).

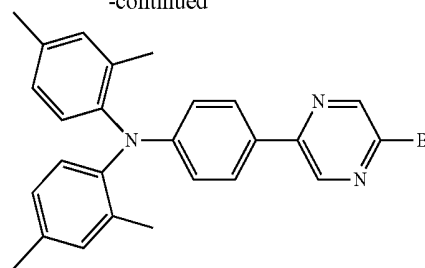


N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)aniline (Compound 17)

[0144] A mixture of N-(4-bromophenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (Compound 16) (15 g, 39.5 mmol), bis(pinacolato)diboron (10.41 g, 41 mmol), KOAc (7.84 g, 80 mmol), Bis(2-diphenylphosphinophenyl)ether (3.23 g, 6 mmol) and Pd(OAc)₂ (0.44 g, 2 mmol) in dioxane (100 mL) was degassed and heated at about 100° C. overnight. The resulting mixture was poured into ethyl acetate (200 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/ethyl acetate 18:1. After removal of solvents, a white solid (Compound 17) was obtained (14 g, in 83% yield).



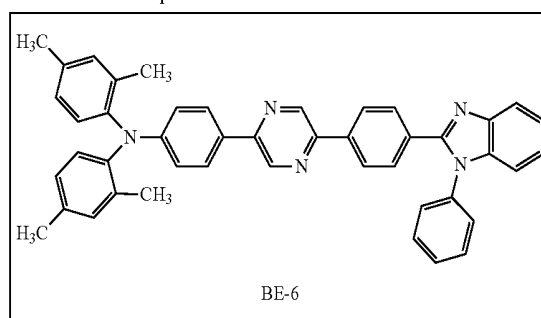
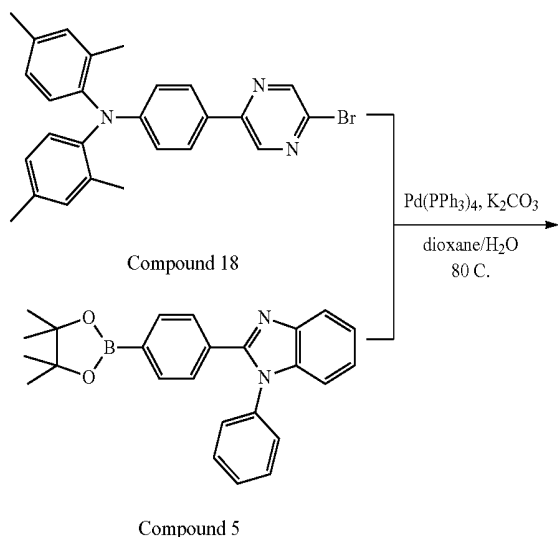
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Compound 18

N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (Compound 18)

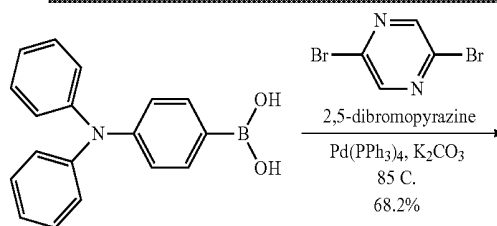
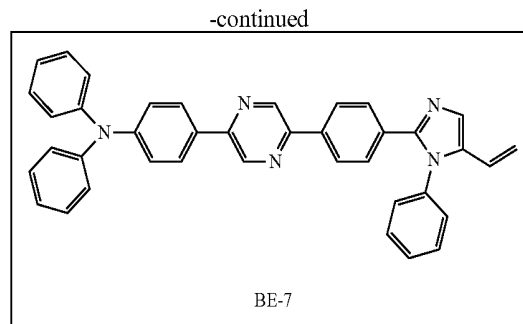
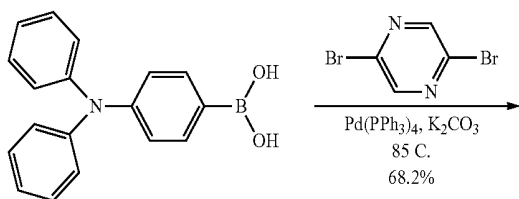
[0145] A mixture of N-(2,4-dimethylphenyl)-2,4-dimethyl-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)aniline (Compound 17) (6.0 g, 14 mmol), 2,5-dibromopyrazine (7.74 g, 30 mmol), Pd(PPh₃)₄ (0.5 g, 0.43 mmol), K₂CO₃ (4.14 g, 30 mmol) in dioxane/water (80 mL/17 mL) was degassed and heated at about 80° C. overnight. The resulting mixture was poured into ethyl acetate (200 mL), washed with brine, dried over Na₂SO₄, then loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1 to 6:1 to 7:3. The desired yellow fraction was collected, and a yellow solid (Compound 18) was obtained after removal of solvents (3.83 g, 60% yield).



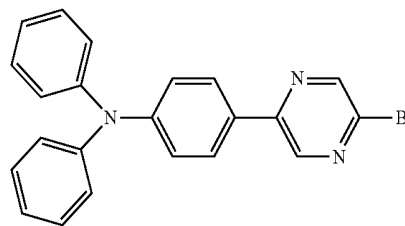
Compound BE-6

[0146] A mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(2,4-dimethylphenyl)-2,4-dimethylaniline (Compound 18) (1.67 g, 3.65 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (Compound 5) (1.445 g, 3.65 mmol), Pd(PPh₃)₄ (0.21 g, 0.18 mmol), K₂CO₃ (0.966 g, 7 mmol) in dioxane/water (50 mL/10 mL) was degassed and heated at about 100° C. overnight. The resulting mixture was poured into ethyl acetate (200 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 1:1 to dichloromethane to dichloromethane/ethyl acetate 90:5. The desired yellow fraction was collected. After removal of solvent, a yellow solid (BE-6) was obtained (2.2 g, in 93% yield). Confirmed by LCMS (APCI+): calcd for C₄₅H₃₈N₅ (M+H): 648; Found: 648.

Synthesis of BE-7



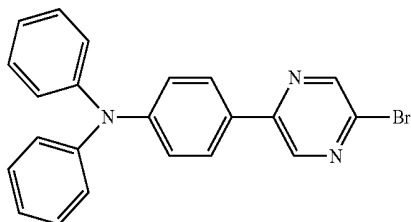
(4-(diphenylamino)
phenyl)boronic acid



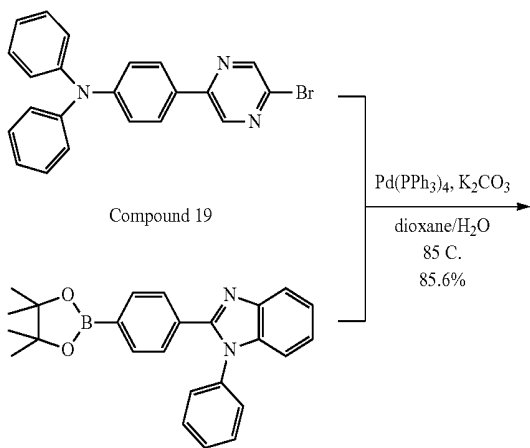
Compound 19

4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline
(Compound 19)

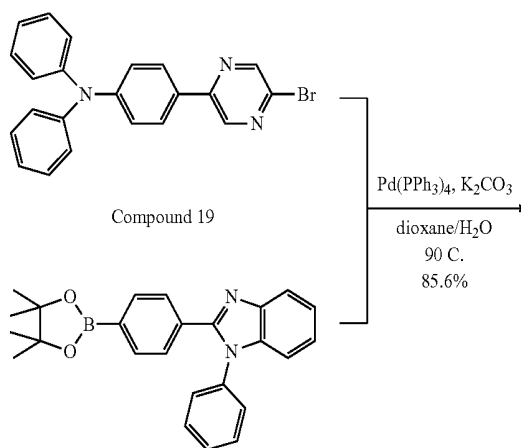
[0147] A mixture of (4-(diphenylamino)phenyl)boronic acid (3.26 g, 11.3 mmol), 2,5-dibromopyrazine (5.82 g, 22.6 mmol), Pd(PPh₃)₄ (0.635 g, 0.55 mmol), K₂CO₃ (3.45 g, 25 mmol) in dioxane/water (100 mL/16 mL) was degassed and heated at about 85° C. for about 20 hours. The resulting mixture was poured into ethyl acetate (250 mL), washed with brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1. After removal of solvent, a yellow solid (Compound 19) was obtained (3.1 g, in 68.2% yield).



Compound 19

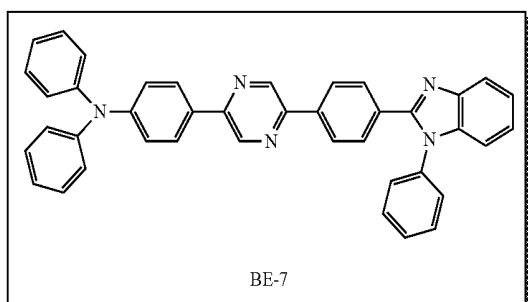


Compound 5



Compound 5

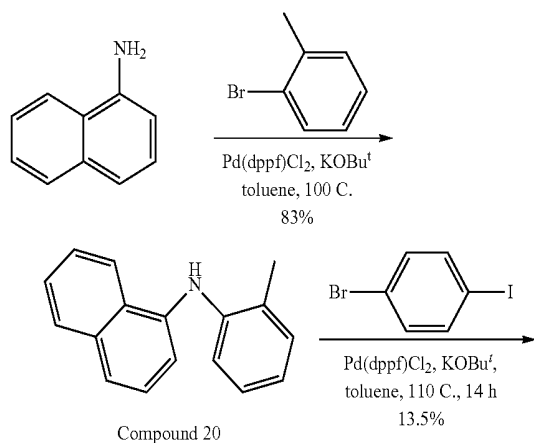
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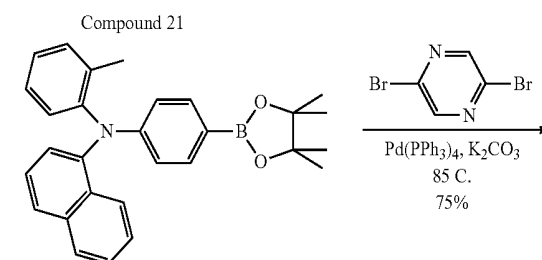
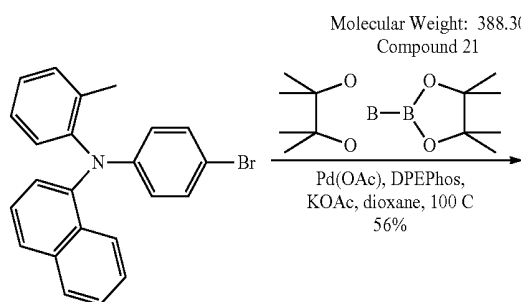
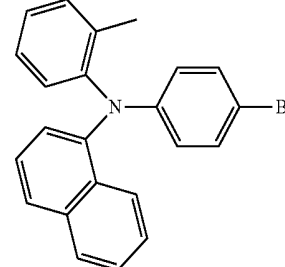
Compound BE-7

[0148] A mixture of 4-(5-bromopyrazin-2-yl)-N,N-diphenylaniline (Compound 19) (1.54 g, 3.83 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzo[d]imidazole (Compound 5) (1.52 g, 3.83 mmol), Pd(PPh₃)₄ (0.22 g, 0.19 mmol), K₂CO₃ (1.104 g, 8 mmol) in dioxane/water (100 mL/15 mL) was degassed and heated at about 90° C. for about 16 hours. The resulting mixture was poured into ethyl acetate (250 mL), washed with brine, concentrated and yellow precipitate formed. Filtration and washing with ethyl acetate gave a solid and filtrate. The filtrate was loaded on silica gel and purified by flash column using eluents of hexanes to dichloromethane to dichloromethane/ethyl acetate (9:1 to 4:1). The desired fraction was collected. The solid from the filtration was dissolved in dichloromethane, purified by flash column using eluents of hexanes to dichloromethane to dichloromethane/ethyl acetate 9:1. The desired fraction was collected. Both desired fractions from the chromatography were combined, after removal of solvent, the solid was recrystallized in dichloromethane/ethyl acetate to give a yellow solid (BE-7), 1.94 g in 85.6% yield. Confirmed by LCMS (APCI+): calcd for C₄₁H₃₀N₅ (M+H): 592; found: 592.

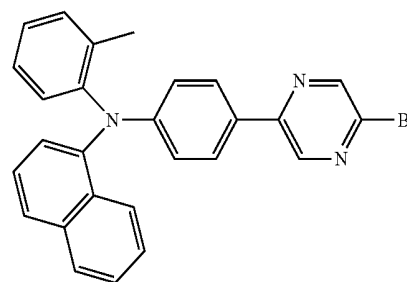
Synthesis of BE-8

[0149]

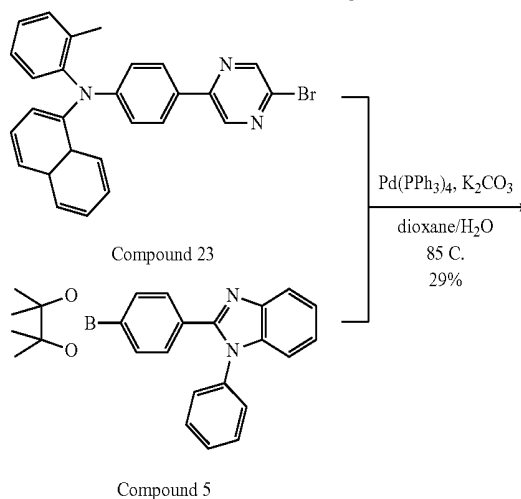
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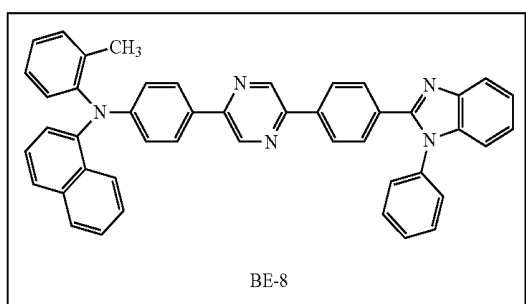
Compound 22



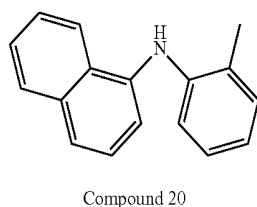
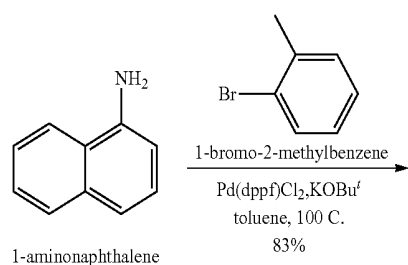
Compound 23



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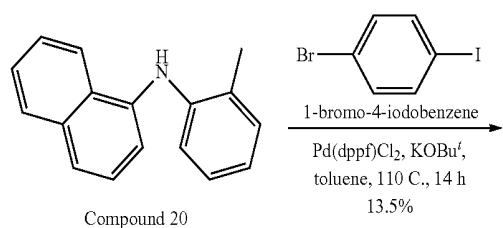


Molecular Weight: 655.79

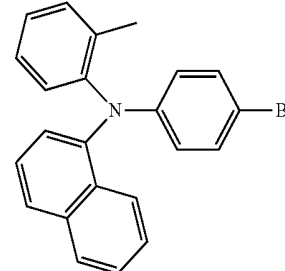


N-(o-tolyl)naphthalen-1-amine (Compound 20)

[0150] A mixture of 1-aminonaphthalene (7.15 g, 50 mmol), 1-bromo-2-methylbenzene (8.5 g, 50 mmol), Pd(dppf)Cl₂ (1.0 g, 1.36 mmol), sodium tert-butoxide (9.6 g, 0.1 mol) in toluene (120 mL) was degassed and heated at about 100° C. overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. After removal of solvents, an oil (Compound 20) was obtained, 10.2 g in 91.5% yield.



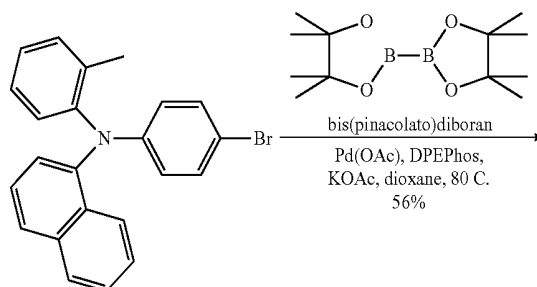
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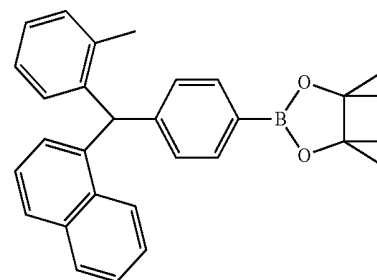
Compound 21

N-(4-bromophenyl)-N-(o-tolyl)naphthalen-1-amine
(Compound 21)

[0151] A mixture of N-(o-tolyl)naphthalen-1-amine (Compound 20) (2.0 g, 8.6 mmol), 1-bromo-4-iodobenzene (8.67 g, 30 mmol), Pd(dppf)Cl₂ (0.365 g, 0.5 mmol), potassium tert-butoxide (1.96 g, 20 mmol) in toluene was degassed and heated at 110° C. overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na₂SO₄, loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 9:1. After removal of solvents, a yellow solid (Compound 21) was obtained, 0.45 g in 13.5% yield.



Compound 21

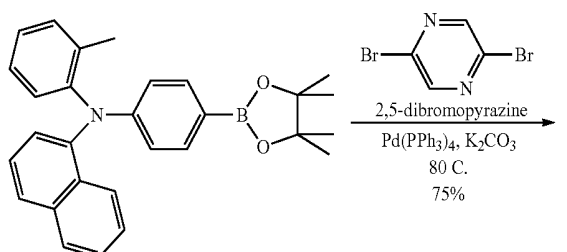


Compound 22

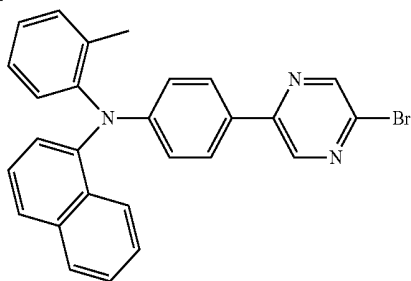
N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine
(Compound 22)

[0152] A mixture of N-(4-bromophenyl)-N-(o-tolyl)naphthalen-1-amine (Compound 21) (0.87 g, 2.24 mmol), bis(pinacolato)diboron (0.635 g, 2.5 mmol), Pd(dppf)Cl₂ (81.8 mg, 0.11 mmol), KOAc (0.49 g, 5 mmol) in dioxane (50 mL) was degassed and heated at 80° C. overnight. The resulting mix-

ture was worked up with ethyl acetate/brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/ethyl acetate 18:1. After removal of solvents, a yellow solid (Compound 22) was obtained, 0.55 g in 56% yield.



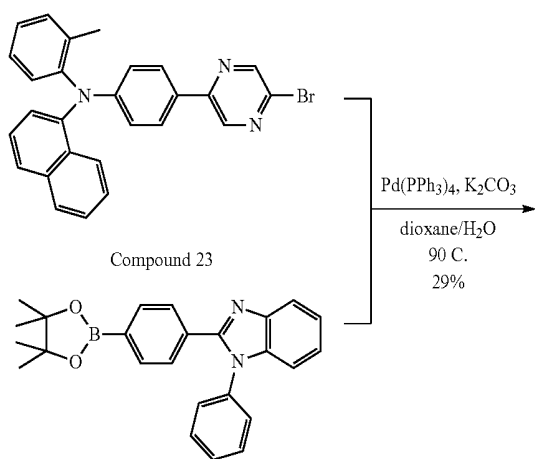
Compound 22



Compound 23

N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (Compound 23)

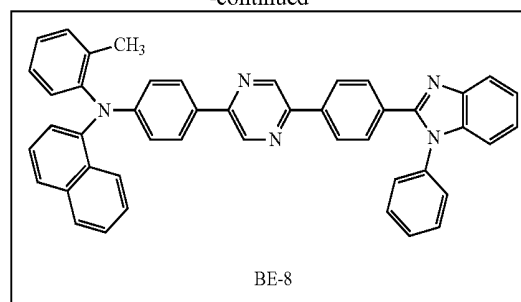
[0153] A mixture of N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (Compound 22) (0.55 g, 1.26 mmol), 2,5-dibromopyrazine (0.77 g, 3.0 mmol), $\text{Pd}(\text{PPh}_3)_4$ (0.1 g, 0.09 mmol), K_2CO_3 (0.414 g, 3 mmol) in dioxane/water (40 mL/8 mL) was degassed and heated at 80° C. overnight. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes/dichloromethane 9:1 to 3:2. After removal of solvents, a yellow solid (Compound 23) was obtained, 0.44 g in 75% yield.



Compound 23

Compound 5

-continued



BE-8

Molecular Weight: 655.79

Compound BE-8

[0154] A mixture of N-(4-(5-bromopyrazin-2-yl)phenyl)-N-(o-tolyl)naphthalen-1-amine (Compound 23) (0.44 g, 0.94 mmol), 1-phenyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1H-benzod[imidazole] (Compound 5) (0.374 g, 0.94 mmol), $\text{Pd}(\text{PPh}_3)_4$ (0.058 g, 0.05 mmol), K_2CO_3 (0.276 g, 2 mmol) in dioxane/water (40 mL/8 mL) was degassed and heated at about 90° C. for 5 hours. The resulting mixture was worked up with ethyl acetate/brine, dried over Na_2SO_4 , loaded on silica gel and purified by flash column using eluents of hexanes to hexanes/dichloromethane 4:1 to 1:1 to dichloromethane/ethyl acetate 10:1. The desired fraction was collected, after removal of solvents, the solid was recrystallized in dichloromethane/hexanes to give a yellow solid (BE-8), 0.18 g in 29% yield. Confirmed by LCMS (APCI+): calcd for $\text{C}_{46}\text{H}_{34}\text{N}_5$ (M+H): 656; Found: 656.

Example of OLED Device Configuration and Performance

Example 2

[0155] ITO coated glass substrates will be cleaned by ultrasound in water, 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) will be spin-coated at 3000 rpm onto the pre-cleaned and O_2 -plasma treated (ITO)-substrate and annealed at about 180° C. for 30 min, to yield a thickness of around 55 nm. In a glove-box hosted vacuum deposition system at a pressure of 10^{-7} torr (1 torr=133.322 Pa), DTASi will be first deposited on top of PEDOT/PSS layer at deposition rate of 0.06 nm/s, yielding a 30 nm thick film. Then the BE-2 will be heated and deposited on top of DTASi, yielding about a 5 nm thick film, followed by co-deposition of BE-2 and Ir(PIQ)₂(acac) at deposition rates of about 0.06 nm/s to form a 5 nm thick layer, and deposition of another BE-2 layer having a thickness of about 5 nm. Then 1,3,5-tris(N-phenylbenzimidazo1-2-yl)benzene (TPBI) at deposition rate around 0.06 nm/s will be deposited on the BE-2 layer to form a 40 nm thick film. LiF (1.0 nm) and Al (100 nm) will be then deposited successively at deposition rates of 0.005 and 0.2 nm/s, respectively. Each individual device will have areas of 0.14 cm^2 .

Example 3

[0156] All spectra will be measured with an Ocean Optics HR 4000 spectrometer and I-V-L characteristics were taken

with a Keithley 2400 SourceMeter and Newport 2832-C power meter and 818 UV detector. All device operation will be performed inside a nitrogen-filled glove-box. An example of a configuration of the device (Device-A) is shown in FIG. 4.

[0157] It is anticipated that upon determining the luminescent efficiency and power efficiency as a function of luminance of Device-A, a plot of the electroluminescence spectrum of Device-A, and the CRI of Device A, BE-2 will be suitable as a host material in hybrid OLED devices.

[0158] Unless otherwise indicated, all numbers expressing quantities of ingredients, properties such as molecular weight, reaction conditions, and so forth used in the specification and claims are to be understood as being modified in all instances by the term “about.” Accordingly, unless indicated to the contrary, the numerical parameters set forth in the specification and attached claims are approximations that may vary depending upon the desired properties sought to be obtained. At the very least, and not as an attempt to limit the application of the doctrine of equivalents to the scope of the claims, each numerical parameter should at least be construed in light of the number of reported significant digits and by applying ordinary rounding techniques.

[0159] The terms “a,” “an,” “the” and similar referents used in the context of describing the invention (especially in the context of the following claims) are to be construed to cover both the singular and the plural, unless otherwise indicated herein or clearly contradicted by context. All methods described herein can be performed in any suitable order unless otherwise indicated herein or otherwise clearly contradicted by context. The use of any and all examples, or exemplary language (e.g., “such as”) provided herein is intended merely to better illuminate the invention and does not pose a limitation on the scope of any claim. No language in the specification should be construed as indicating any non-claimed element essential to the practice of the invention.

[0160] Groupings of alternative elements or embodiments disclosed herein are not to be construed as limitations. Each group member may be referred to and claimed individually or in any combination with other members of the group or other elements found herein. It is anticipated that one or more members of a group may be included in, or deleted from, a group for reasons of convenience and/or patentability. When any such inclusion or deletion occurs, the specification is deemed to contain the group as modified thus fulfilling the written description of all Markush groups used in the appended claims.

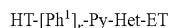
[0161] Certain embodiments are described herein, including the best mode known to the inventors for carrying out the invention. Of course, variations on these described embodiments will become apparent to those of ordinary skill in the art upon reading the foregoing description. The inventor expects skilled artisans to employ such variations as appropriate, and the inventors intend for the invention to be practiced otherwise than specifically described herein. Accordingly, the claims include all modifications and equivalents of the subject matter recited in the claims as permitted by applicable law. Moreover, any combination of the above-described elements in all possible variations thereof is contemplated unless otherwise indicated herein or otherwise clearly contradicted by context.

[0162] In closing, it is to be understood that the embodiments disclosed herein are illustrative of the principles of the claims. Other modifications that may be employed are within

the scope of the claims. Thus, by way of example, but not of limitation, alternative embodiments may be utilized in accordance with the teachings herein. Accordingly, the claims are not limited to embodiments precisely as shown and described.

1-12. (canceled)

13. A compound represented by a formula:



wherein HT is optionally substituted diphenylamine or optionally substituted phenyl(naphthyl)amine,

each Ph^1 is independently optionally substituted p-phenylene, wherein the p-phenylene directly bonded to HT may optionally form a bond to a phenyl of HT to form a three ring system;

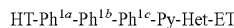
Py is optionally substituted pyrazin-2,5-ylene;

Het is optionally substituted p-phenylene or optionally substituted pyridin-2,5-ylene;

ET is optionally substituted benzimidazol-2-yl, optionally substituted benzoxazol-2-yl, or optionally substituted benzothiazol-2-yl; and

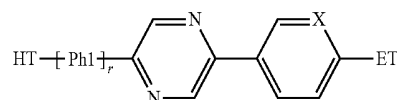
r is 1, 2, 3.

14. The compound of claim 1, further represented by a formula:



wherein Ph^{1a} is optionally substituted p-phenylene, or HT-Ph^{1a} is 9-phenylcarbazol-3-yl; and Ph^{1b} and Ph^{1c} are independently a bond or optionally substituted p-phenylene.

15. The compound of claim 13, further represented by a formula:

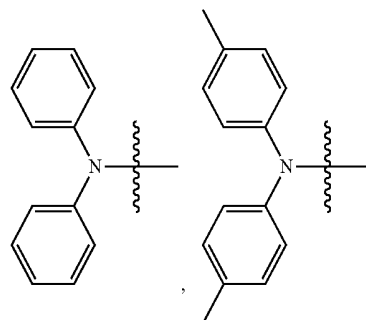


wherein X is C or N.

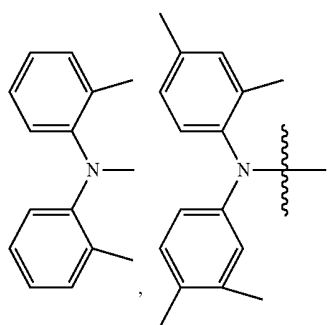
16. The compound of claim 13, wherein r is 1.

17. The compound of claim 13, wherein ET is optionally substituted 1-phenyl-1H-benzo[d]imidazol-2-yl.

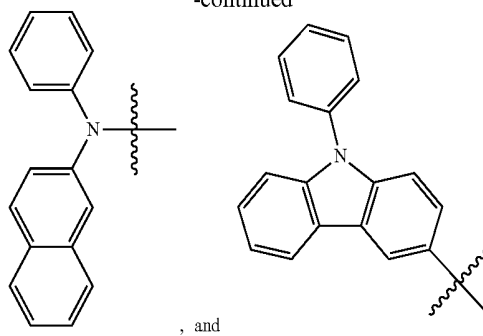
18. The compound of claim 13, wherein HT is



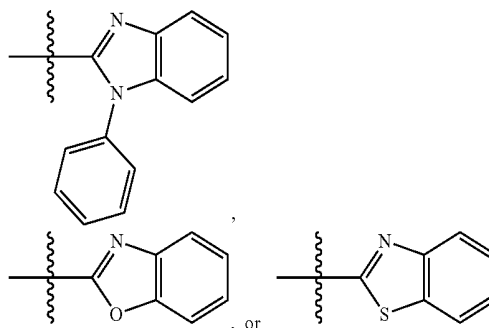
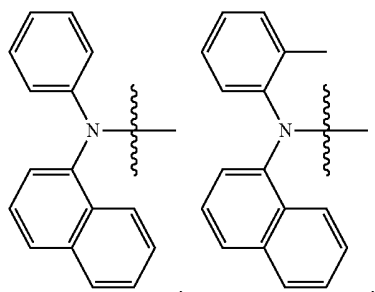
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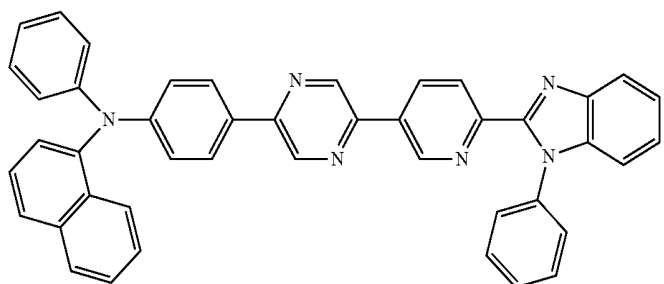
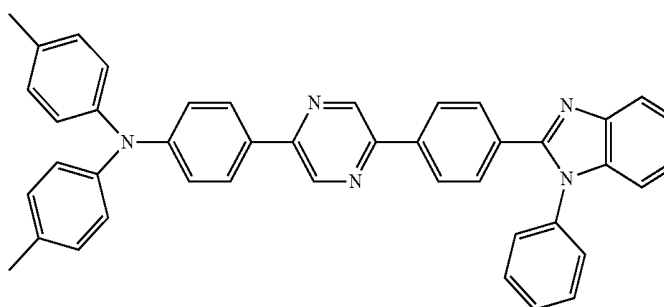
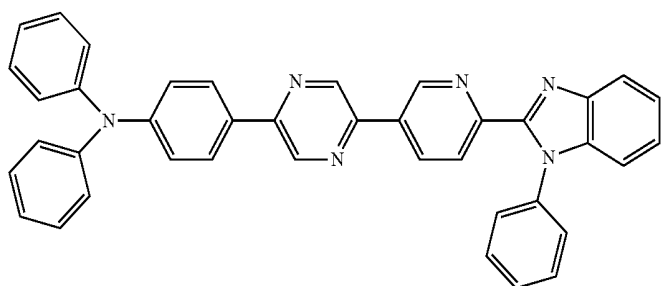
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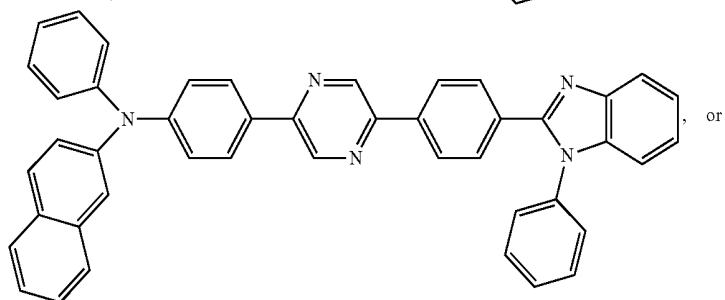
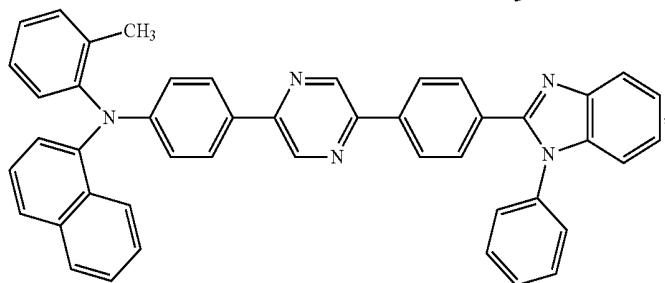
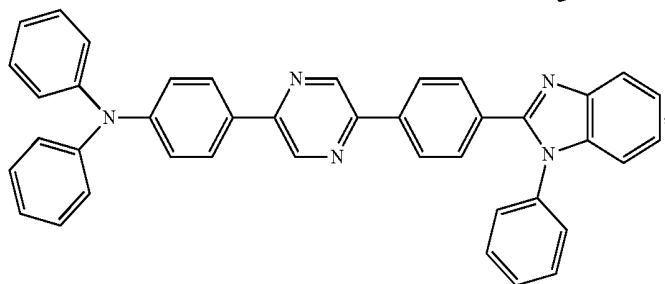
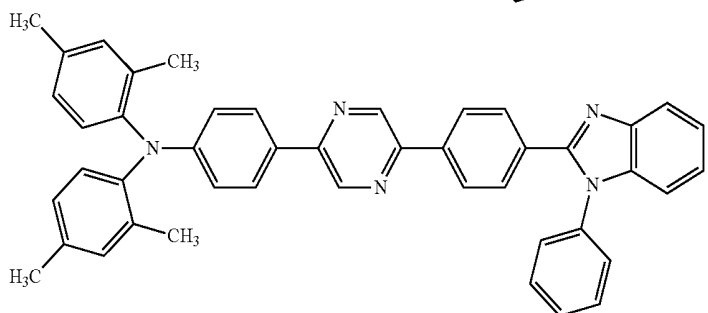
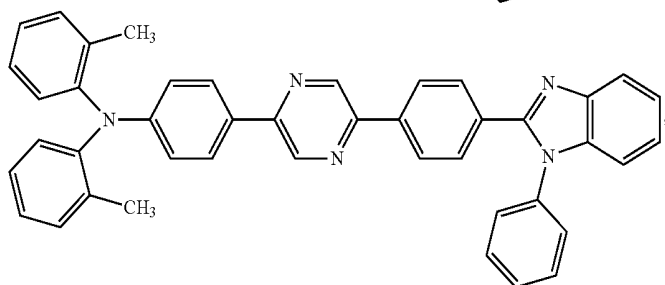
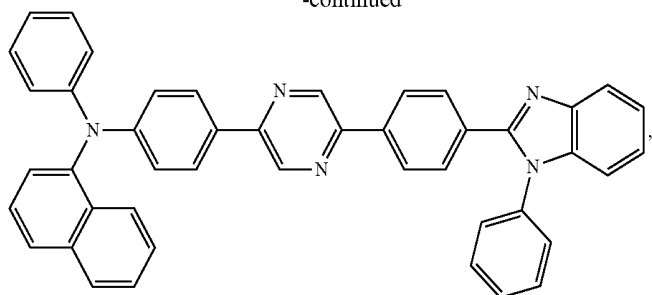
19. The compound of claim 13, wherein ET is



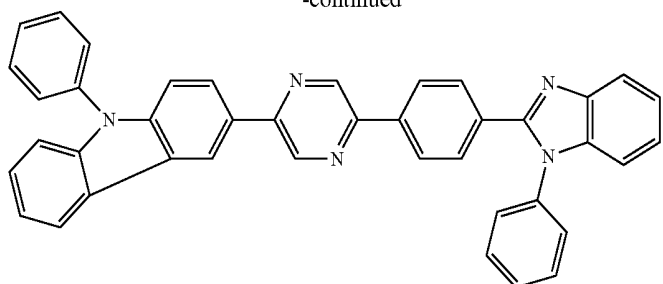
20. The compound of claim 13, wherein the compound is:



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21. The compound of claim 13, wherein the compound is electroluminescent.

22. The compound of claim 21, wherein the compound has a lowest energy triplet having an energy of about 2.5 eV to about 4 eV.

23. A light emitting layer comprising the compound of claim 13.

24. 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 comprising an compound of claim 13.

25. The compound of claim 13, wherein Het is optionally substituted p-phenylene.

26. The compound of claim 13, wherein Het is optionally substituted pyridin-2,5-ylene.

27. The compound of claim 13, wherein r is 2.

28. The compound of claim 13, wherein r is 3.

* * * * *

专利名称(译)	有机发光主体材料		
公开(公告)号	US20140159015A1	公开(公告)日	2014-06-12
申请号	US14/102138	申请日	2013-12-10
[标]申请(专利权)人(译)	日东电工株式会社		
申请(专利权)人(译)	日东电工株式会社		
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摘要(译)

由式表示的化合物等杂芳基芳基化合物可用于电子器件如有机发光器件中。例如，该化合物可用作发光层中的发光材料。

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