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Ma et al.

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(54) **TRIPHENYLENE-BENZOFURAN/ BENZOTHIOPHENE/BENZOSELENOPHENE COMPOUNDS WITH SUBSTITUENTS JOINING TO FORM FUSED RINGS**

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C07D 307/77	(2006.01)
C07D 333/50	(2006.01)
C09K 11/06	(2006.01)
H01L 51/00	(2006.01)
H05B 33/20	(2006.01)
H05B 33/22	(2006.01)
H01L 51/50	(2006.01)

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

CPC ***C09K 11/06*** (2013.01); ***H01L 51/0054*** (2013.01); ***H05B 33/20*** (2013.01); ***H05B 33/22*** (2013.01); *C09K 2211/1088* (2013.01); *C09K 2211/1092* (2013.01); *C09K 2211/1096* (2013.01); *H01L 51/0072* (2013.01); *H01L 51/0074* (2013.01); *H01L 51/5012* (2013.01)

USPC **428/690**; 549/42; 549/41; 549/456; 549/457

(58) **Field of Classification Search**

None

See application file for complete search history.

(56) **References Cited**

U.S. PATENT DOCUMENTS

4,769,292	A	9/1988	Tang et al.
5,061,569	A	10/1991	VanSlyke et al.
5,247,190	A	9/1993	Friend et al.
5,703,436	A	12/1997	Forrest et al.
5,707,745	A	1/1998	Forrest et al.

(Continued)

FOREIGN PATENT DOCUMENTS

EP	0650955	5/1995
EP	1725079	11/2006

(Continued)

OTHER PUBLICATIONS

Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, (1998).

(Continued)

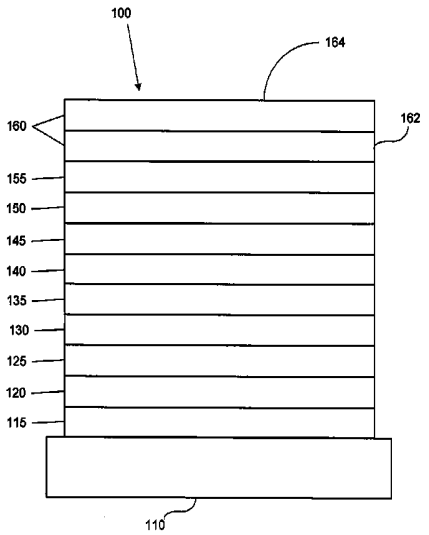
Primary Examiner — J. L. Yang

(74) *Attorney, Agent, or Firm* — Duane Morris LLP

(57) **ABSTRACT**

Compounds comprising a triphenylene moiety and a benzo- or dibenzo-moiety are provided. In particular, the benzo- or dibenzo-moiety has a fused substituent. These compounds may be used in organic light emitting devices, particularly in combination with yellow, orange and red emitters, to provide devices with improved properties.

19 Claims, 3 Drawing Sheets



(56) **References Cited**

U.S. PATENT DOCUMENTS

5,834,893	A	11/1998	Bulovic et al.	
5,844,363	A	12/1998	Gu et al.	
6,013,982	A	1/2000	Thompson et al.	
6,087,196	A	7/2000	Sturm et al.	
6,091,195	A	7/2000	Forrest et al.	
6,097,147	A	8/2000	Baldo et al.	
6,294,398	B1	9/2001	Kim et al.	
6,303,238	B1	10/2001	Thompson et al.	
6,337,102	B1	1/2002	Forrest et al.	
6,468,819	B1	10/2002	Kim et al.	
6,528,187	B1	3/2003	Okada	
6,687,266	B1	2/2004	Ma et al.	
6,835,469	B2	12/2004	Kwong et al.	
6,921,915	B2	7/2005	Takiguchi et al.	
7,087,321	B2	8/2006	Kwong et al.	
7,090,928	B2	8/2006	Thompson et al.	
7,154,114	B2	12/2006	Brooks et al.	
7,250,226	B2	7/2007	Tokito et al.	
7,279,704	B2	10/2007	Walters et al.	
7,332,232	B2	2/2008	Ma et al.	
7,338,722	B2	3/2008	Thompson et al.	
7,393,599	B2	7/2008	Thompson et al.	
7,396,598	B2	7/2008	Takeuchi et al.	
7,431,968	B1	10/2008	Shtein et al.	
7,445,855	B2	11/2008	Mackenzie et al.	
7,534,505	B2	5/2009	Lin et al.	
2002/0034656	A1	3/2002	Thompson et al.	
2002/0134984	A1	9/2002	Igarashi	
2002/0158242	A1	10/2002	Son et al.	
2003/0136657	A1	7/2003	Eckert et al.	
2003/0152802	A1	8/2003	Tsuboyama et al.	
2003/0162053	A1	8/2003	Marks et al.	
2003/0175553	A1	9/2003	Thompson et al.	
2003/0230980	A1	12/2003	Forrest et al.	
2004/0036077	A1	2/2004	Ise	
2004/0076853	A1*	4/2004	Jarikov	428/690
2004/0137267	A1	7/2004	Igarashi et al.	
2004/0137268	A1	7/2004	Igarashi et al.	
2004/0174116	A1	9/2004	Lu et al.	
2005/0025993	A1	2/2005	Thompson et al.	
2005/0112407	A1	5/2005	Ogasawara et al.	
2005/0238919	A1	10/2005	Ogasawara	
2005/0244673	A1	11/2005	Satoh et al.	
2005/0260441	A1	11/2005	Thompson et al.	
2005/0260449	A1	11/2005	Walters et al.	
2005/1026044		11/2005	Thompson at al.	
2006/0008670	A1	1/2006	Lin et al.	
2006/0202194	A1	9/2006	Jeong et al.	
2006/0240279	A1	10/2006	Adamovich et al.	
2006/0251923	A1	11/2006	Lin et al.	
2006/0263635	A1	11/2006	Ise	
2006/0280965	A1	12/2006	Kwong et al.	
2006/1028096		12/2006	Kwong at al.	
2007/0190359	A1	8/2007	Knowles et al.	
2007/0278938	A1	12/2007	Yabunouchi et al.	
2008/0015355	A1	1/2008	Schafer et al.	
2008/0018221	A1	1/2008	Egen et al.	
2008/0106190	A1	5/2008	Yabunouchi et al.	
2008/0124572	A1	5/2008	Mizuki et al.	
2008/0220265	A1	9/2008	Xia et al.	
2008/0297033	A1	12/2008	Knowles et al.	
2009/0008605	A1	1/2009	Kawamura et al.	
2009/0009065	A1	1/2009	Nishimura et al.	
2009/0017330	A1	1/2009	Iwakuma et al.	
2009/0030202	A1	1/2009	Iwakuma et al.	
2009/0039776	A1	2/2009	Yamada et al.	
2009/0045730	A1	2/2009	Nishimura et al.	
2009/0045731	A1	2/2009	Nishimura et al.	
2009/0101870	A1	4/2009	Prakash et al.	
2009/0108737	A1	4/2009	Kwong et al.	
2009/0115316	A1	5/2009	Zheng et al.	
2009/0165846	A1	7/2009	Johannes et al.	
2009/0167162	A1	7/2009	Lin et al.	
2009/0179554	A1	7/2009	Kuma et al.	
2010/0237334	A1*	9/2010	Ma et al.	257/40

FOREIGN PATENT DOCUMENTS

EP	2034538	3/2009	
EP	2112214	10/2009	
EP	2 213 641	8/2010	
JP	200511610	1/2005	
JP	2007123392	5/2007	
JP	2007254297	10/2007	
JP	2008074939	10/2009	
WO	WO 0139234	5/2001	
WO	WO 0202714	1/2002	
WO	WO 0215645	2/2002	
WO	WO 03040257	5/2003	
WO	WO 03060956	7/2003	
WO	WO 2004093207	10/2004	
WO	WO 2004107822	12/2004	
WO	WO 2005014551	2/2005	
WO	WO 2005019373	3/2005	
WO	WO 2005030900	4/2005	
WO	WO 2005089025	9/2005	
WO	WO 2005123873	12/2005	
WO	WO 2006009024	1/2006	
WO	WO 2006056418	6/2006	
WO	WO 2006072002	7/2006	
WO	WO 2006082742	8/2006	
WO	WO 2006098120	9/2006	
WO	WO 2006100298	9/2006	
WO	WO 2006103874	10/2006	
WO	WO 2006114966	11/2006	
WO	WO 2006/130598	12/2006	
WO	WO 2006132173	12/2006	
WO	WO 2007002683	1/2007	
WO	WO 2007004380	1/2007	
WO	WO 2007063754	6/2007	
WO	WO 2007063796	6/2007	
WO	WO 2008056746	5/2008	
WO	WO 2008101842	8/2008	
WO	WO 2008132085	11/2008	
WO	WO 2009000673	12/2008	
WO	WO 2009003898	1/2009	
WO	WO 2009008311	1/2009	
WO	WO 2009/021107	2/2009	
WO	WO 2009/021126 A2 *	2/2009	C07D 307/91
WO	WO 2009018009	2/2009	
WO	WO 2009050290	4/2009	
WO	WO 2009/021126	5/2009	
WO	WO 2009021126	5/2009	
WO	WO 2009062578	5/2009	
WO	WO 2009063833	5/2009	
WO	WO 2009066778	5/2009	
WO	WO 2009066779	5/2009	
WO	WO 2009086028	7/2009	
WO	WO 2009100991	8/2009	
WO	WO 2010/036765	4/2010	

OTHER PUBLICATIONS

Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999).

Ashe et al., Heteroatom Chemistry, 5(2), 113-19, 1994.

Tominaga et al., Journal of Heterocyclic Chemistry, 18(5), 967-72, Aug. 1981.

Baldwin et al., Journal of Heterocyclic Chemistry, 21(6), 1775-9, 1984.

Buquet et al., Tetrahedron, 37(1), 75-81, 1981.

U.S. Appl. No. 61/343,402, filed Apr. 28, 2010.

The International Search Report corresponding to the PCT//US2011/034081 application.

Kuwabara, Yoshiyuki et al., "Thermally Stable Multilayered Organic Electroluminescent Devices Using Novel Starburst Molecules, 4,4',4"-Tri(*N*-carbazolyl)triphenylamine (TCTA) and 4,4',4"-Tris(3-methylphenylphenyl-amino)triphenylamine (*m*-MTDATA), as Hole-Transport Materials," *Adv. Mater,* 6(9):677-679 (1994).

Paulose, Betty Marie Jennifer S. et al., "First Examples of Alkenyl Pyridines as Organic Ligands for Phosphorescent Iridium Complexes," *Adv. Mater.,* 16(22):2003-2007 (2004).

(56) **References Cited**

OTHER PUBLICATIONS

Tung, Yung-Liang et al., "Organic Light-Emitting Diodes Based on Charge-Neutral Ru^{II} PHosphorescent Emitters," Adv. Mater., 17(8):1059-1064 (2005).

Huang, Jinsong et al., "Highly Efficient Red-Emission Polymer Phosphorescent Light-Emitting Diodes Based on Two Novel Tris(1-phenylisoquinolinato-C2,*N*)iridium(III) Derivatives," *Adv. Mater.,* 19:739-743 (2007).

Wong, Wai-Yeung, "Multifunctional Iridium Complexes Based on Carbazole Modules as Highly Efficient Electrophosphors," *Angew. Chem. Int. Ed.,* 45:7800-7803 (2006).

Tang, C.W. and VanSlyke, S.A., "Organic Electroluminescent Diodes," *Appl. Phys. Lett.,* 51(12):913-915 (1987).

Adachi, Chihaya et al., "Organic Electroluminescent Device Having a Hole Conductor as an Emitting Layer," *Appl. Phys. Lett.,* 55(15):1489-1491 (1989).

Ma, Yuguang et al., "Triplet Luminescent Dinuclear-Gold(*I*) Complex-Based Light-Emitting Diodes with Low Turn-On voltage," *Appl. Phys. Lett.,* 74(10):1361-1363 (1999).

Gao, Zhiqiang et al., "Bright-Blue Electroluminescence From a Silyl-Substituted ter-(phenylene-vinylene) derivative," *Appl. Phys. Lett.,* 74(6):865-867 (1999).

Lee, Chang-Lyoul et al., "Polymer Phosphorescent Light-Emitting Devices Doped with Tris(2-phenylpyridine) Iridium as a Triplet Emitter," *Appl. Phys. Lett.,* 77(15):2280-2282 (2000).

Hung, L.S. et al., "Anode Modification in Organic Light-Emitting Diodes by Low-Frequency Plasma Polymerization of CHF_3," *Appl. Phys. Lett.,* 78(5):673-675 (2001).

Ikai, Masamichi and Tokito, Shizuo, "Highly Efficient Phosphorescence From Organic Light-Emitting Devices with an Exciton-Block Layer," *Appl. Phys. Lett.,* 79(2):156-158 (2001).

Wang, Y. et al., "Highly Efficient Electroluminescent Materials Based on Fluorinated Organometallic Iridium Compounds," *Appl. Phys. Lett.,* 79(4):449-451 (2001).

Kwong, Raymond C. et al., "High Operational Stability of Electrophosphorescent Devices," *Appl. Phys. Lett.,* 81(1):162-164 (2002).

Holmes, R.J. et al., "Blue Organic Electrophosphorescence Using Exothermic Host-Guest Energy Transfer," *Appl. Phys. Lett.,* 82(15):2422-2424 (2003).

Sotoyama, Wataru et al., "Efficient Organic LIght-Emitting Diodes with Phosphorescent Platinum Complexes Containing N^AC^AN-Coordinating Tridentate Ligand,",*Appl. Phys. Lett.,* 86:153505-1-153505-3 (2005).

Okumoto, Kenji et al., "Green Fluorescent Organic Light-Emitting Device with External Quantum Efficiency of Nearly 10%," *Appl. Phys. Lett.,* 89:063504-1-063504-3 (2006).

Kanno, Hiroshi et al., "Highly Efficient and Stable Red Phosphorescent Organic Light-Emitting Device Using bis[2-(2-benzothiazoyl)phenolato]zinc(II) as host material," *Appl. Phys. Lett.,* 90:123509-1-123509-3 (2007).

Aonuma, Masaki et al., "Material Design of Hole Transport Materials Capable of Thick-Film Formation in Organic Light Emitting Diodes," *Appl. Phys. Lett.,* 90:183503-1-183503-3 (2007).

Sun, Yiru and Forrest, Stephen R., "High-Efficiency White Organic Light Emitting Devices with Three Separate Phosphorescent Emission Layers," *Appl. Phys. Lett.,* 91:263503-1-263503-3 (2007).

Adachi, Chihaya et al., "High-Efficiency Red Electrophosphorescence Devices," *Appl. Phys. Lett.,* 78(11):1622-1624 (2001).

Wong, Keith Man-Chung et al., A Novel Class of Phosphorescent Gold(III) Alkynyl-Based Organic Light-Emitting Devices with Tunable Colour, *Chem. Commun.,* 2906-2908 (2005).

Hamada, Yuji et al., "High Luminance in Organic Electroluminescent Devices with Bis(10-hydroxybenzo[h]quinolinato)beryllium as an Emitter," *Chem. Lett.,* 905-906 (1993).

Nishida, Jun-ichi et al., "Preparation, Characterization, and Electroluminescence Characteristics of α-Diimine-type Platinum(II) Complexes with Perfluorinated Phenyl Groups as Ligands," *Chem. Lett.,* 34(4):592-593 (2005).

Mi, Bao-Xiu et al., "Thermally Stable Hole-Transporting Material for Organic Light-Emitting Diode: an Isoindole Derivative," *Chem. Mater.,* 15(16):3148-3151 (2003).

Huang, Wei-Sheng et al., "Highly Phosphorescent Bis-Cyclometalated Iridium Complexes Containing Benzoimidazole-Based Ligands," *Chem. Mater.,* 16(12):2480-2488 (2004).

Niu, Yu-Hua et al., "Highly Efficient Electrophosphorescent Devices with Saturated Red Emission from a Neutral Osmium Complex," *Chem. Mater.,* 17(13):3532-3536 (2005).

Lo, Shih-Chun et al., "Blue Phosphorescence from Iridium(III) Complexes at Room Temperature," *Chem. Mater.,* 18(21):5119-5129 (2006).

Takizawa, Shin-ya et al., "Phosphorescent Iridium Complexes Based on 2-Phenylimidazo[1,2-α]pyridine Ligands: Tuning of Emission Color toward the Blue Region and Application to Polymer Light-Emitting Devices," *Inorg. Chem.,* 46(10):4308-4319 (2007).

Lamansky, Sergey et al., "Synthesis and Characterization of Phosphorescent Cyclometalated Iridium Complexes," *Inorg. Chem.,* 40(7):1704-1711 (2001).

Ranjan, Sudhir et al., "Realizing Green Phosphorescent Light-Emitting Materials from Rhenium(I) Pyrazolato Diimine Complexes," *Inorg. Chem.,* 42(4):1248-1255 (2003).

Noda, Tetsuya and Shirota,Yasuhiko, "5,5'-Bis(dimesitylbory1)-2,2'-bithiophene and 5,5"-Bis(dimesitylboryl)-2,2':5',2"-terthiophene as a Novel Family of Electron-Transporting Amorphous Molecular Materials," *J. Am. Chem. Soc.,* 120 (37):9714-9715 (1998).

Sakamoto, Youichi et al., "Synthesis, Characterization, and Electron-Transport Property of Perfluorinated Phenylene Dendrimers," *J. Am. Chem. Soc.,* 122(8):1832-1833 (2000).

Adachi, Chihaya et al., "Nearly 100% Internal Phosphorescence Efficiency in an Organic Light Emitting Device," *J. Appl. Phys.,* 90(10):5048-5051 (2001).

Shirota, Yasuhiko et al., "Starburst Molecules Based on π-Electron Systems as Materials for Organic Electroluminescent Devices," *Journal of Luminescence*, 72-74:985-991 (1997).

Inada, Hiroshi and Shirota, Yasuhiko, "1,3,5-Tris[4-(diphenylamino)phenyl]benzene and its Methylsubstituted Derivatives as a Novel Class of Amorphous Molecular Materials," *J. Mater. Chem.,* 3(3):319-320 (1993).

Kido, Junji et al., 1,2,4-Triazole Derivative as an Electron Transport Layer in Organic Electroluminescent Devices, *Jpn. J. Appl. Phys.,* 32:L917-L920 (1993).

Van Slyke, S. A. et al., "Organic Electroluminescent Devices with Improved Stability," *Appl. Phys. Lett.,* 69(15):2160-2162 (1996).

Guo, Tzung-Fang et al., "Highly Efficient Electrophosphorescent Polymer Light-Emitting Devices," *Organic Electronics,* 1:15-20 (2000).

Palilis, Leonidas C., "High Efficiency Molecular Organic Light-Emitting Diodes Based on Silole Derivatives and Their Exciplexes," *Organic Electronics*, 4:113-121 (2003).

Ikeda, Hisao et al., "P-185: Low-Drive-Voltage OLEDs with a Buffer Layer Having Molybdenum Oxide," *SID Symposium Digest*, 37:923-926 (2006).

T. Östergård et al., "Langmuir-Blodgett Light-Emitting Diodes of Poly(3-Hexylthiophene): Electro-Optical Characteristics Related to Structure," *Synthetic Metals*, 87:171-177 (1997).

Hu, Nan-Xing et al., "Novel High T_g Hole-Transport Molecules Based on Indolo[3,2-*b*]carbazoles for Organic Light-Emitting Devices," *Synthetic Metals*, 111-112:421-424 (2000).

Salbeck, J. et al., "Low Molecular Organic Glasses for Blue Electroluminescence," *Synthetic Metals,* 91:209-215 (1997).

* cited by examiner

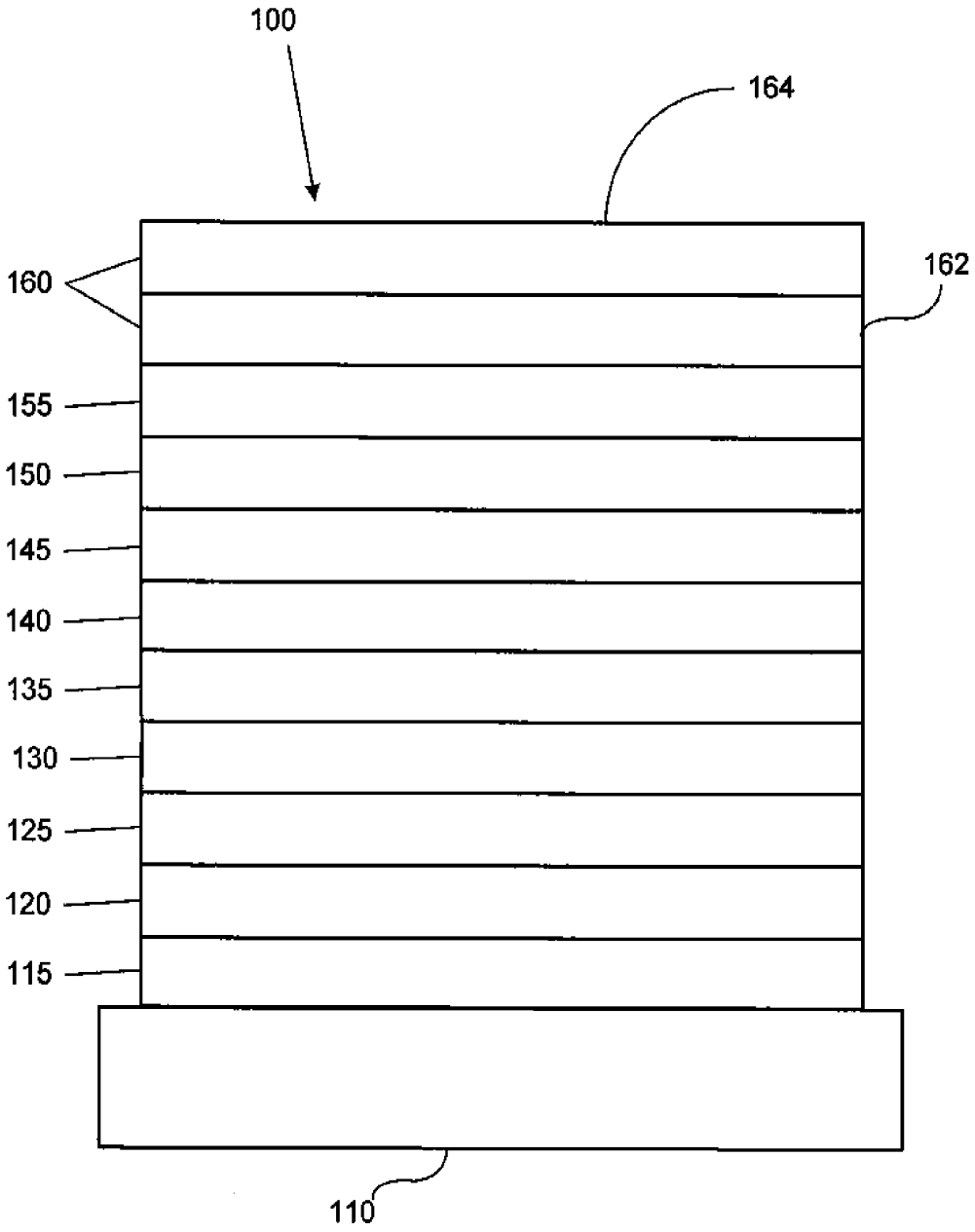


FIGURE 1

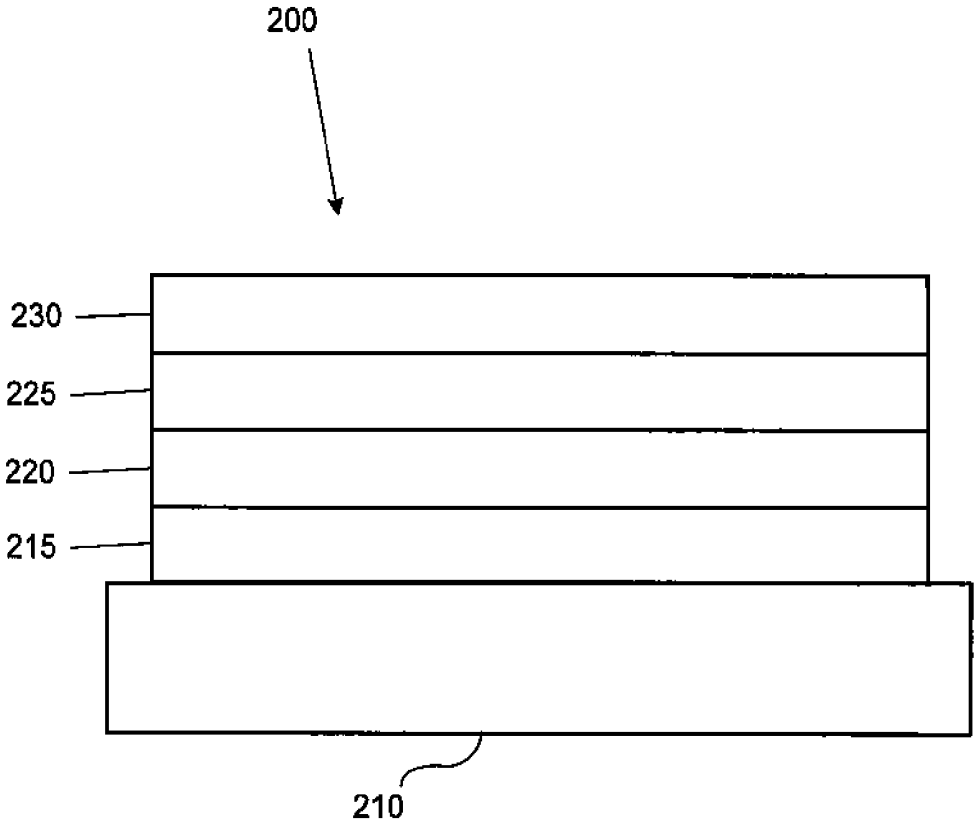
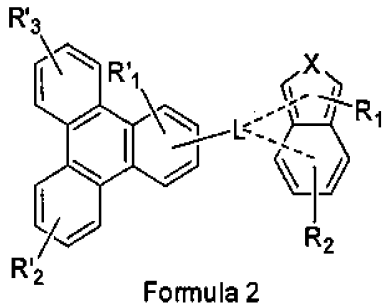


FIGURE 2



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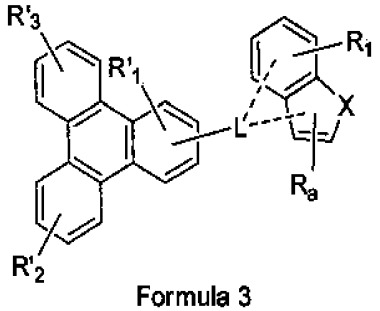
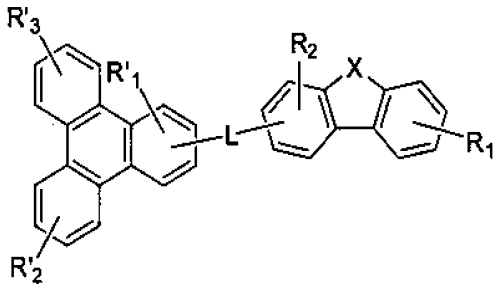


Formula 3



Formula 4

FIGURE 3

TRIPHENYLENE-BENZOFURAN/ BENZOTHIOPHENE/BENZOSELENOPHENE COMPOUNDS WITH SUBSTITUENTS JOINING TO FORM FUSED RINGS

This application claims priority to U.S. Provisional Application Ser. No. 61/343,402, filed Apr. 28, 2010, the disclosure of which is herein expressly incorporated by reference in its entirety.

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

FIELD OF THE INVENTION

The present invention relates to organic light emitting devices (OLEDs). More specifically, the present invention relates to phosphorescent materials comprising a triphenylene moiety and a benzofuran, dibenzofuran, benzothiophene, dibenzothiophene, benzoselenophene or dibenzoselenophene moiety. These materials may provide devices having improved performance.

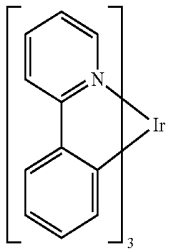
BACKGROUND

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

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

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

One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted $Ir(ppy)_3$, which has the structure:



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

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

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

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

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

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

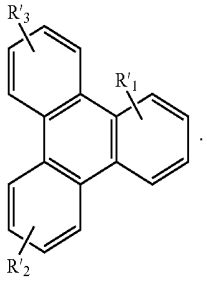
As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum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

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

SUMMARY OF THE INVENTION

Compounds comprising a triphenylene moiety and a benzo- or dibenzo-furan, benzo- or dibenzo-thiophene, or benzo- or dibenzo-selenophene moiety with fused substituents are provided. The compounds comprise the formula:

Formula I

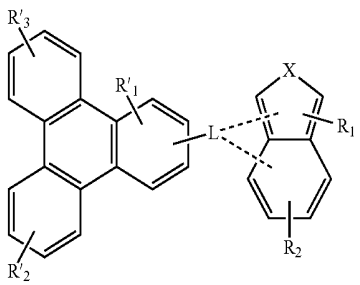


R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R'_1, R'_2, and R'_3 may represent mono, di, tri, or tetra substituents. The compound further comprises a benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety further comprising an additional aromatic or heteroaromatic ring fused to a benzo ring of the benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety.

In one aspect, the aromatic or heteroaromatic ring is a 6-membered carbocyclic or heterocyclic. In another aspect, the aromatic ring is a benzene ring.

In one aspect, the compound is selected from the group consisting of

Formula 2



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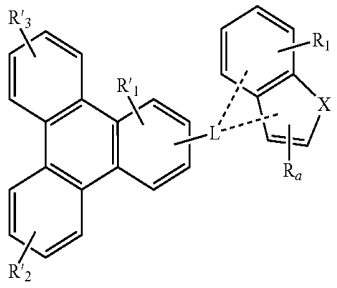
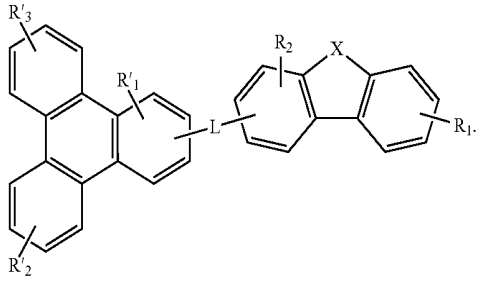
Formula 3



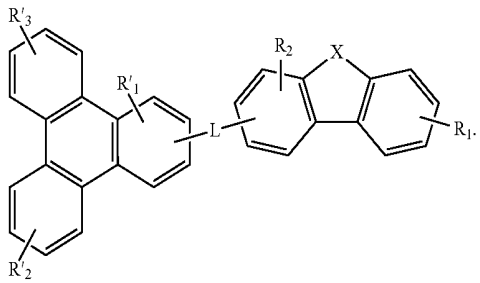
Formula 4



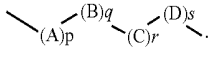
X is O, S or Se. In one aspect, X is S. In another aspect, X is O. R_1, R_2, and R_a are independently selected from hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R_1 and R_2 may represent mono, di, tri or tetra substituents. At least two substituents of R_1 or R_2 are joined to form a fused ring. R_1 represents mono or di substituents which cannot fuse to form a benzo ring. L represents a spacer or a direct connection to the benzofuran, dibenzofuran, benzothiophene, dibenzothiophene, benzoselenophene or benzoselenophene moiety with additional fused rings.

Preferably, the compound has the formula:

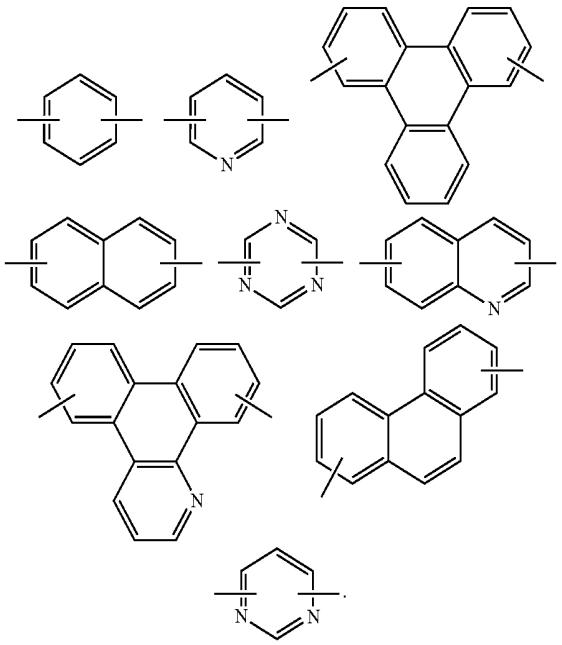
Formula 4



In one aspect, L is a direct connection. In another aspect, L is a spacer having the formula:

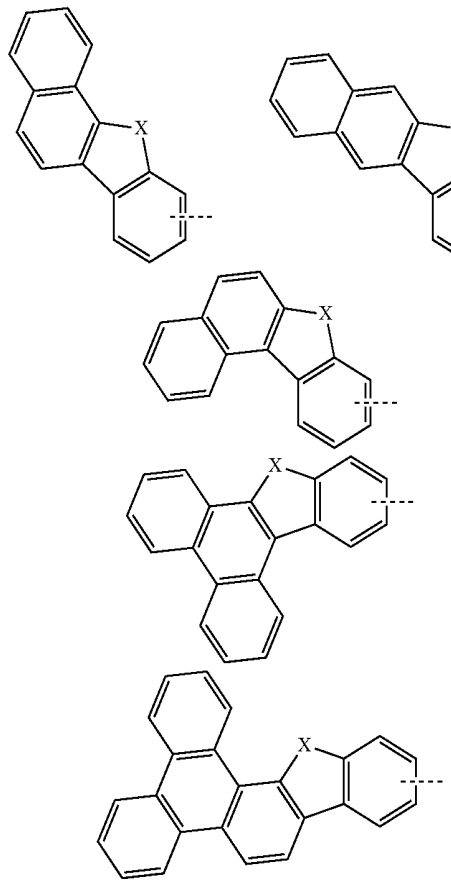


A, B, C and D are independently selected from the group consisting of:



A, B, C and D are optionally further substituted with R_a. Each of p, q, r and s are 0, 1, 2, 3, or 4. p+q+r+s is at least 1. Preferably, L is phenyl.

In one aspect, the benzofuran, dibenzofuran, benzothiophene, dibenzothiophene, benzoselenophene, or dibenzoselenophene moiety with additional fused rings is selected from the group consisting of:



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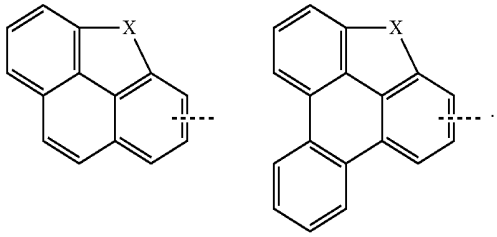


Examples of the compounds are provided, and include compounds selected from the group consisting of Formula 4-1 through Formula 4-28.

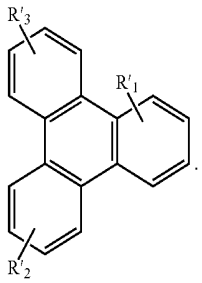
X is O, S or Se. R_1, R_2, R_3, R_4, R_5, R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R_1, R_2, R_3, R_4, R_5, R'_1, R'_2, and R'_3 may represent mono, di, tri or tetra substituents. L is a spacer or a direct linkage.

Specific examples of the compounds provided, include compounds selected from the group consisting of Compound 1-Compound 69.

X is O, S, or Se.

Additionally, a first device comprising an organic light emitting device is provided. The organic light emitting device further comprises an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprises a compound comprising the formula:

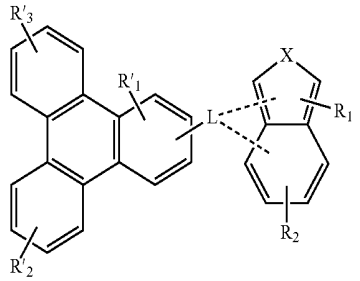
Formula I



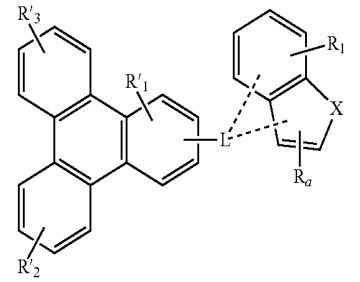
R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R'_1, R'_2, and R'_3 may represent mono, di, tri, or tetra substituents. The compound further comprises a benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety further comprising an additional aromatic or heteroaromatic ring fused to a benzo ring of the benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety.

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

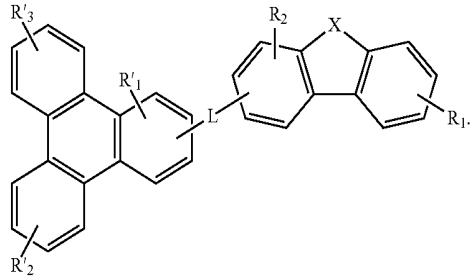
Formula 2



Formula 3

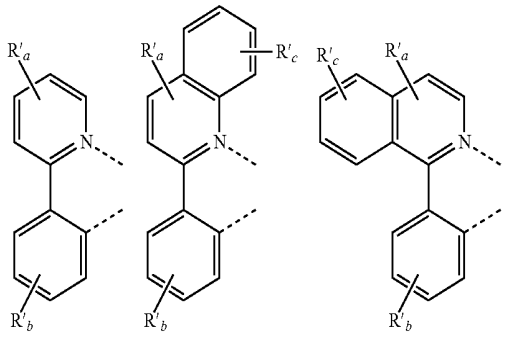


Formula 4



X is O, S or Se. R_1, R_2, and R_a are independently selected from hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R_1 and R_2 may represent mono, di, tri or tetra substituents. At least two substituents of R_1 or R_2 are joined to form a fused ring. R_a represents mono or di substituents which cannot fuse to form a benzo ring. L represents a spacer or a direct connection to the benzofuran, benzothiophene, or benzoselenophene moiety with additional fused rings.

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



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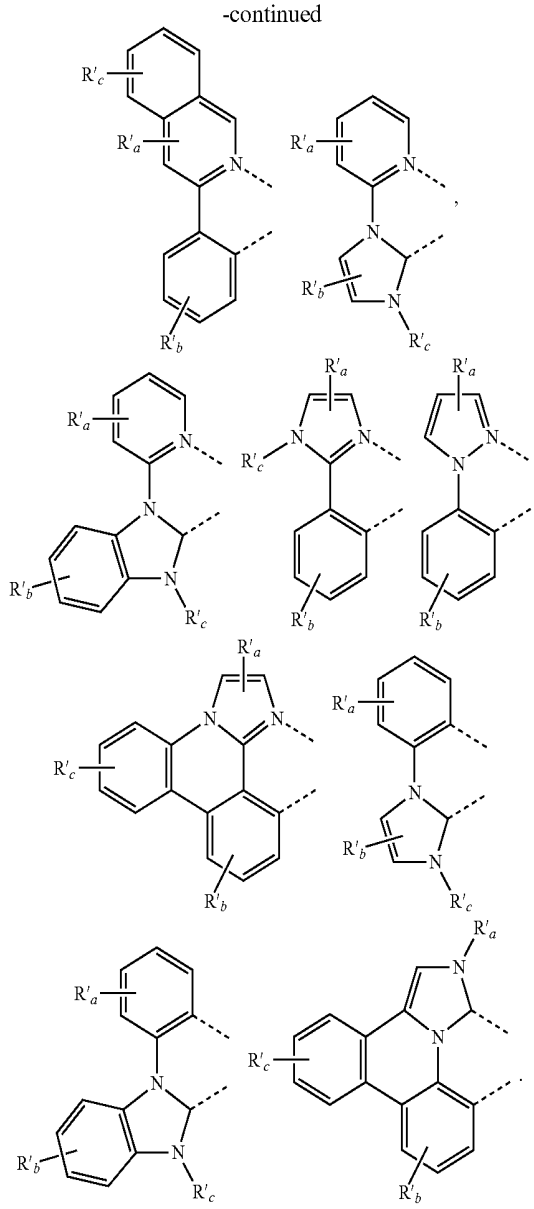


Each of R'_1, R'_b and R'_c may represent mono, di, tri, or tetra substituents. Each of R'_a, R'_b and R'_c are independently selected from a group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, or heteroaryl. Two adjacent substituents may form into a ring.

In another aspect, the device comprises a second organic layer that is non-emissive, and the compound comprising Formula I is a non-emissive material in the second organic layer.

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

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. **1** shows an organic light emitting device.

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

FIG. **3** shows compounds comprising a triphenylene moiety and a benzo- or dibenzo-moiety further substituted with a fused substituent.

DETAILED DESCRIPTION

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

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

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

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

More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F.sub.4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

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

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

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

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. patent application Ser. No. 10/233,470, which is incorporated by reference in its entirety. Other suitable deposition methods

include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processibility than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

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

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

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

Compounds are provided, comprising a triphenylene-containing benzo-fused furan, thiophene or selenophene. Triphenylene is a polyaromatic hydrocarbon with high triplet energy, yet high π-conjugation and a relatively small energy difference between the first singlet and first triplet levels. This suggests that triphenylene has relatively easily accessible HOMO and LUMO levels compared to other aromatic compounds with similar triplet energy (e.g., biphenyl). The advantage of using triphenylene and its derivatives as hosts is that it can accommodate red, green and even blue phosphorescent dopants to give high efficiency without energy quenching. Triphenylene hosts may be used to provide high efficiency and stability PHOLEDs. See Kwong and Alleyene, Triphenylene Hosts in Phosphorescent Light Emitting Diodes, US 2006/0280965, which is herein expressly incorporated by reference in its entirety.

Benzo-fused thiophenes may be used as hole transporting organic conductors. In addition, the triplet energies of benzothiophenes, namely dibenzo[b,d]thiophene (referred to herein as "dibenzothiophene"), benzo[b]thiophene and benzo[c]thiophene are relatively high.

Compounds having a combination of benzo-fused thiophenes and triphenylene may be beneficially used as hosts in PHOLEDs. More specifically, benzo-fused thiophenes are typically more hole transporting than electron transporting, while triphenylene is more electron transporting than hole transporting. Therefore, combining these two moieties in one molecule may offer improved charge balance, which may improve device performance in terms of lifetime, efficiency and low voltage.

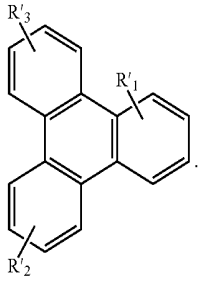
Different chemical linkage of the two moieties can be used to tune the properties of the resulting compound to make it the most appropriate for a particular phosphorescent emitter, device architecture, and/or fabrication-process. For example, m-phenylene linkage is expected to result in higher triplet energy and higher solubility whereas p-phenylene linkage is expected to result in lower triplet energy and lower solubility.

Similar to the characterization of benzo-fused thiophenes, benzo-fused furans are also typically hole transporting materials having relatively high triplet energy. Examples of benzo-fused furans include benzofuran and dibenzofuran. Therefore, a material containing both triphenylene and benzofuran may be advantageously used as host or hole blocking material in PHOLED. A compound containing both of these two groups may offer improved electron stabilization which may improve device stability and efficiency by lowering the voltage. The properties of the triphenylene containing benzofuran compounds may be tuned as necessary by using different chemical linkages to link the triphenylene and the benzofuran.

It has been reported that organic light emitting devices containing compounds with a triphenylene moiety and a benzofuran, benzothiophene, or benzoselenophene moiety provide good performance and stability. See, e.g., WO2009021126 and WO2010036765. Devices incorporating triphenylene-benzofuran/benzothiophene/benzoselenophene with additional fused rings may also show good performance and stability, particularly if the fused rings are aromatic or heteroaromatic rings, because the aromatic fused rings increase the conjugation of the compound, leading to more extended π-electron delocalization and stabilization of charge in the oxidized or reduced state of the molecule.

Compounds comprising a triphenylene moiety and a benzo- or dibenzo-furan, benzo- or dibenzo-thiophene, or benzo- or dibenzo-selenophene moiety with fused substituents are provided (illustrated in FIG. **3**). The compounds comprise the formula:

Formula I



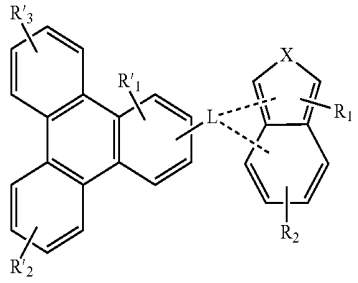
R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R'_1, R'_2, and R'_3 may represent mono, di, tri, or tetra substituents. The

compound further comprises a benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety further comprising an additional aromatic or heteroaromatic ring fused to a benzo ring of the benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety.

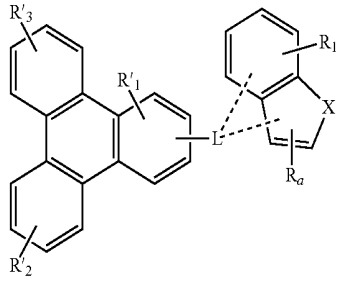
In one aspect, the aromatic or heteroaromatic ring is a 6-membered carbocyclic or heterocyclic. In another aspect, the aromatic ring is a benzene ring.

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

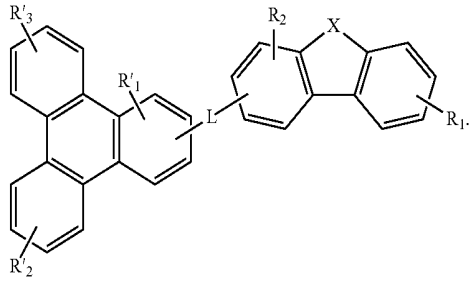
Formula 2



Formula 3



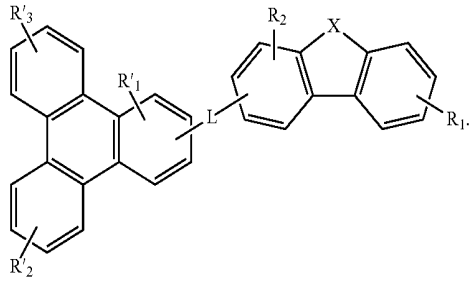
Formula 4



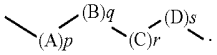
X is O, S or Se. In one aspect, X is S. In another aspect, X is O. R_1, R_2, and R_a are independently selected from hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R_1 and R_2 may represent mono, di, tri or tetra substituents. At least two substituents of R_1 or R_2 are joined to form a fused ring. R_a represents mono or di substituents which cannot fuse to form a benzo ring. L represents a spacer or a direct connection to the benzofuran, benzothiophene, or benzoselenophene moiety with additional fused rings.

Preferably, the compound has the formula:

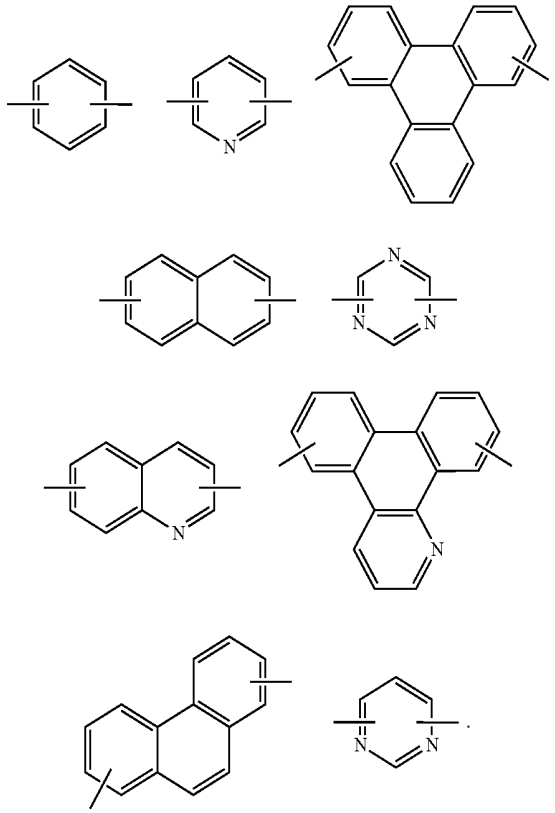
Formula 4



In one aspect, L is a direct connection. In another aspect, L is a spacer having the formula:

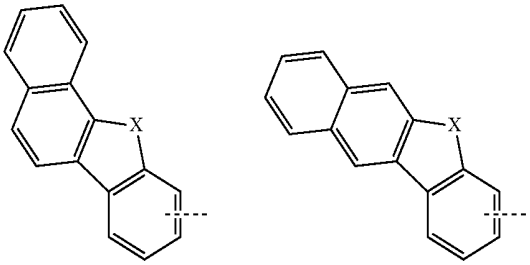


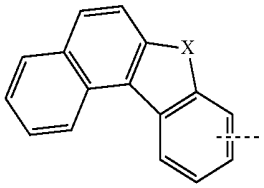
A, B, C and D are independently selected from the group consisting of:

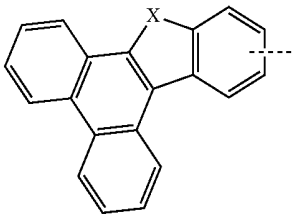


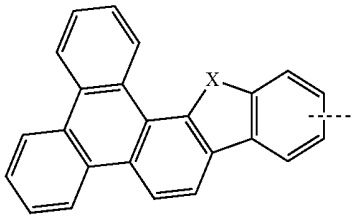
A, B, C and D are optionally further substituted with R_a. Each of p, q, r and s are 0, 1, 2, 3, or 4. p+q+r+s is at least 1. Preferably, L is phenyl.

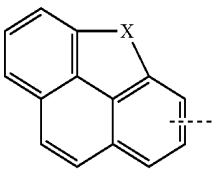
In one aspect, the benzofuran, benzothiophene, or benzoselenophene moiety with additional fused rings is selected from the group consisting of:

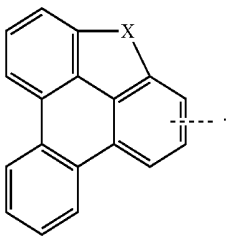






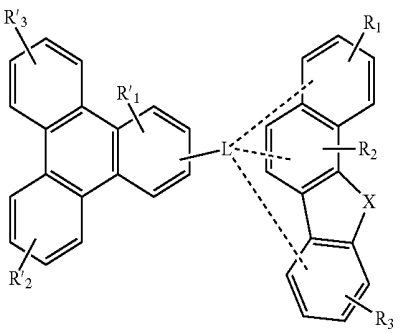






Examples of the compounds are provided, and include compounds selected from the group consisting of:

Formula 4-1



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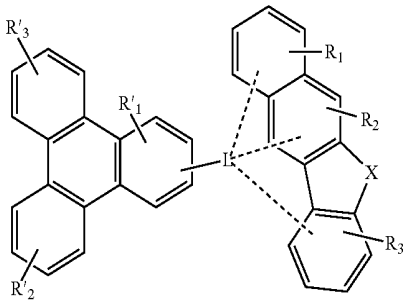
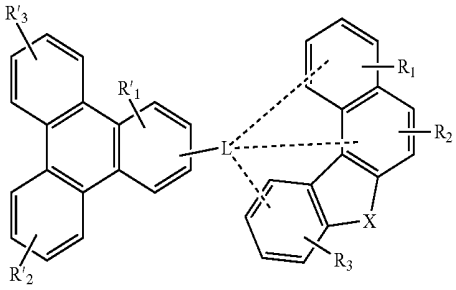
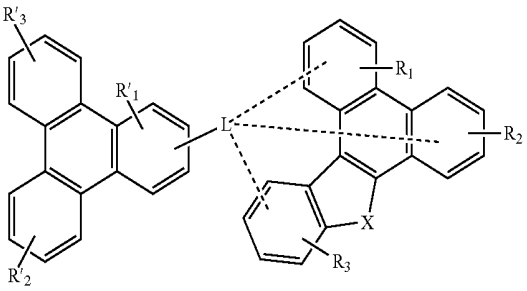
Formula 4-2



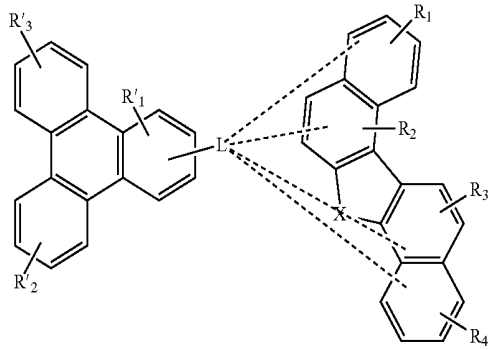
Formula 4-3



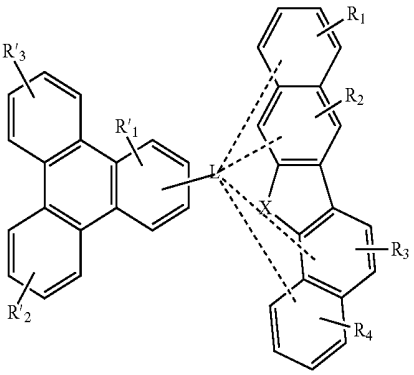
Formula 4-4



Formula 4-5



Fromula 4-6



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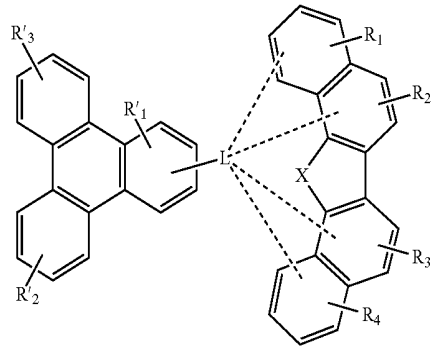
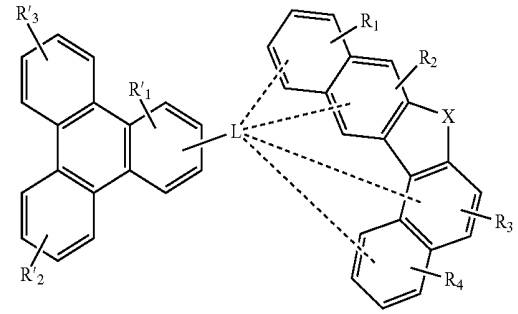
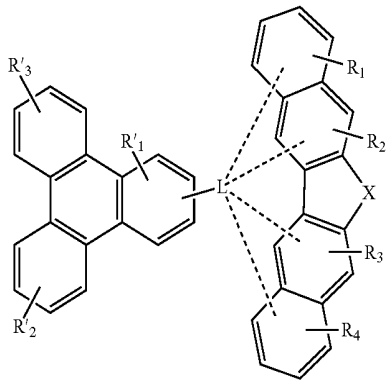
Formula 4-7



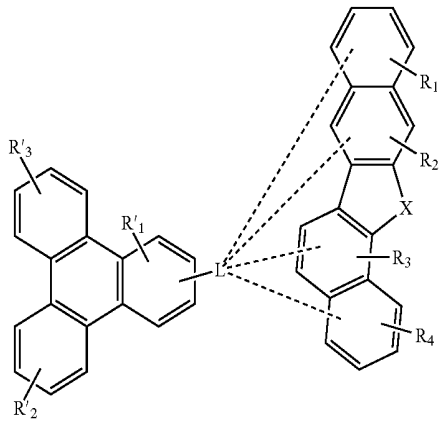
Formula 4-8



Formula 4-9



Formula 4-10



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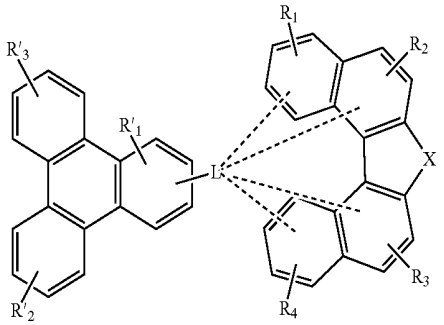
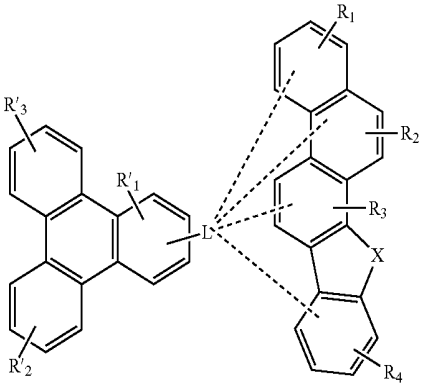
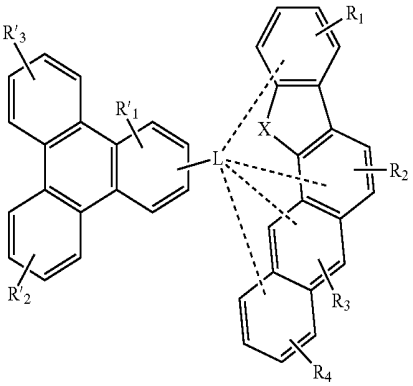
Formula 4-11



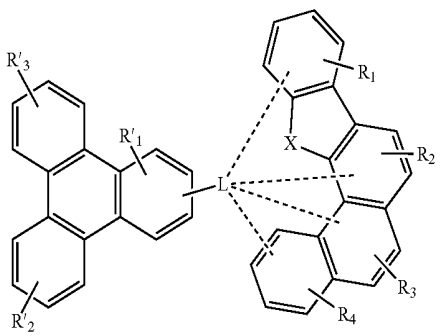
Formula 4-12



Formula 4-13



Formula 4-14



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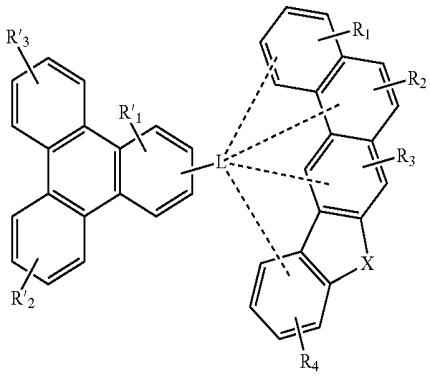
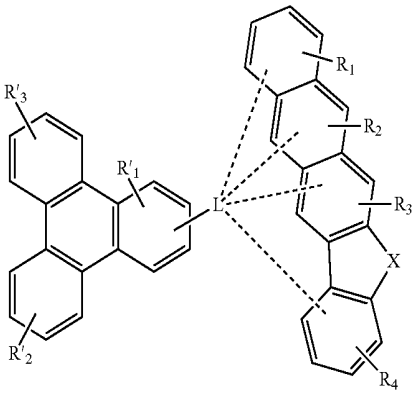
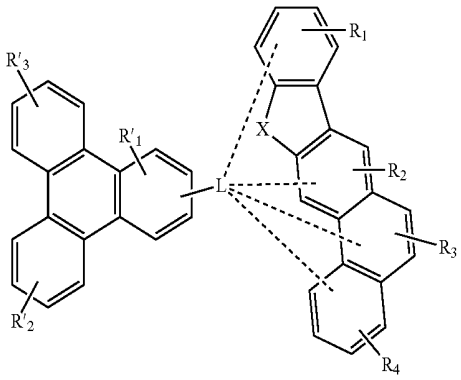
Formula 4-15



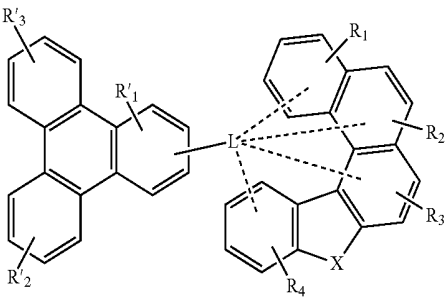
Formula 4-16



Formula 4-17



Formula 4-18



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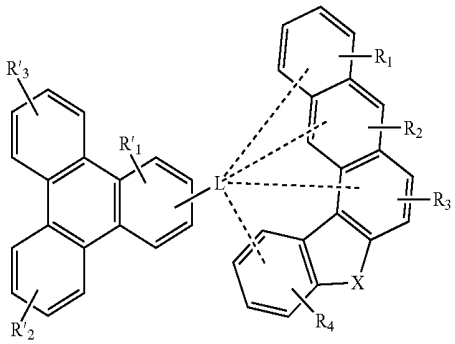
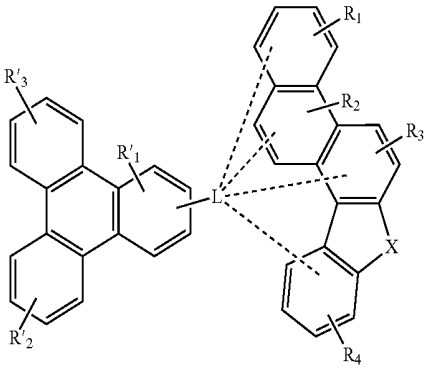
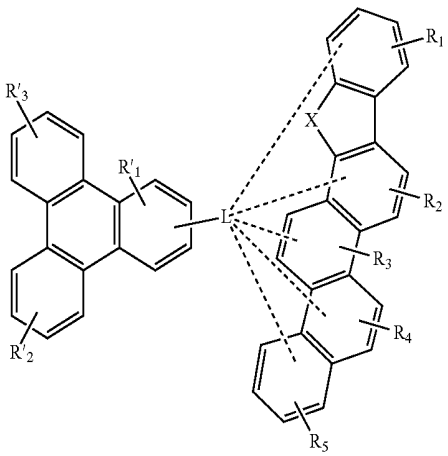
Formula 4-19



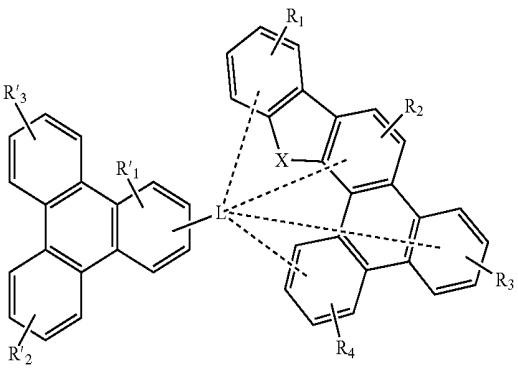
Formula 4-20



Formula 4-21



Formula 4-22



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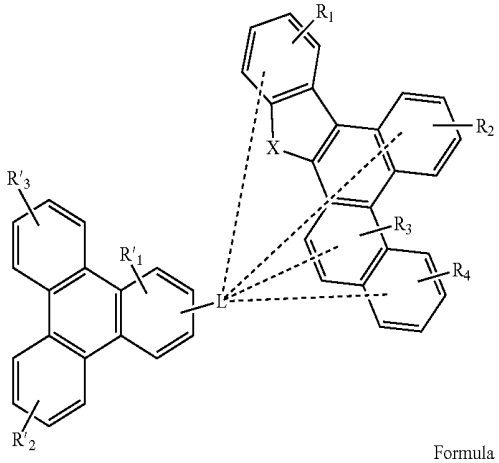
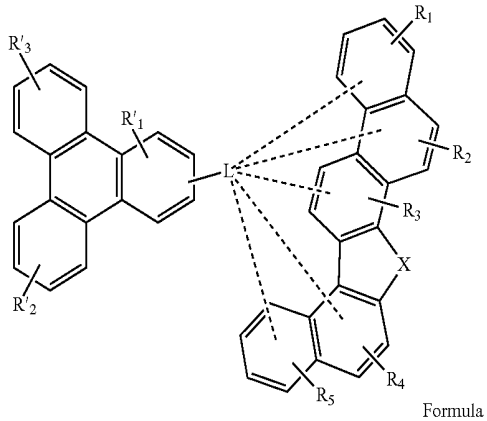
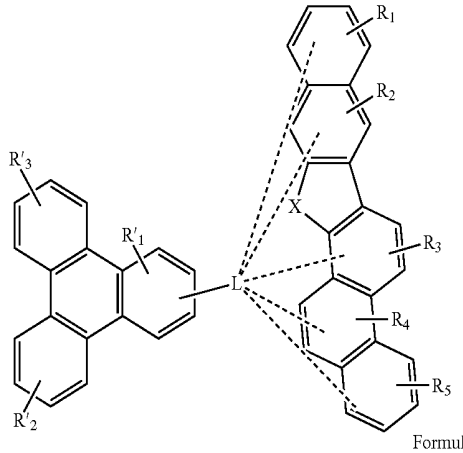
Formula 4-23



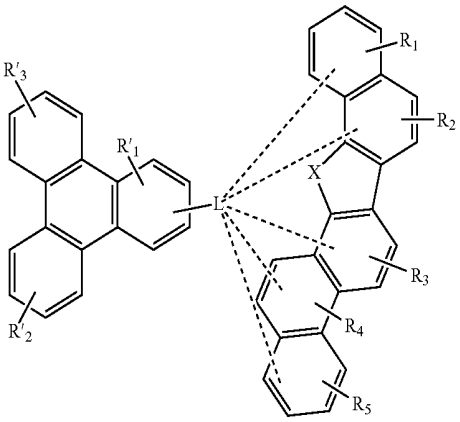
Formula 4-24



Formula 4-25



Formula 4-26



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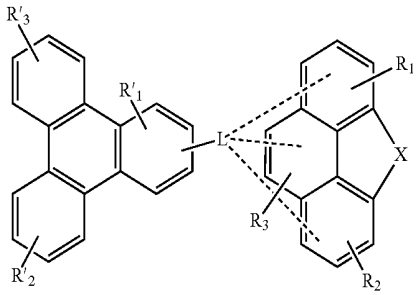
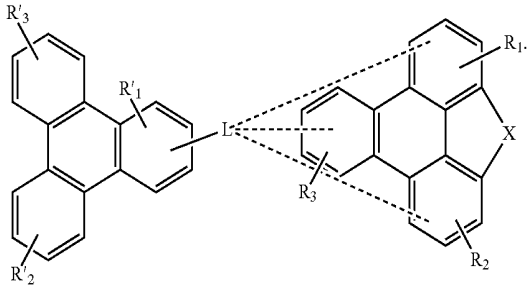
Formula 4-27



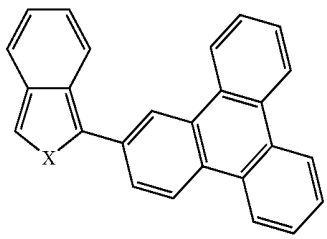
Formula 4-28



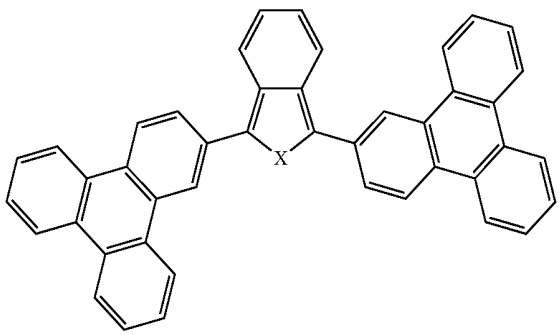
X is O, S or Se. R_1, R_2, R_3, R_4, R_5, R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R_1, R_2, R_3, R_4, R_5, R'_1, R'_2, and R'_3 may represent mono, di, tri or tetra substituents. L is a spacer or a direct linkage.

Specific examples of the compounds provided, include compounds selected from the group consisting of:

Compound 1



Compound 2



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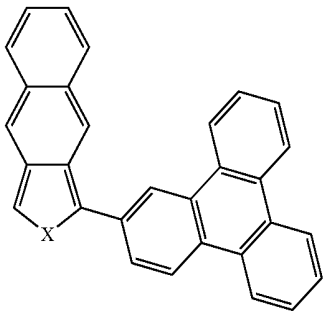
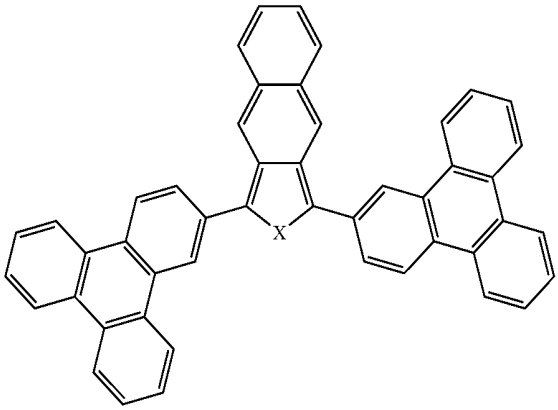
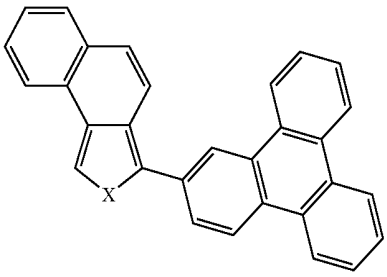
Compound 3



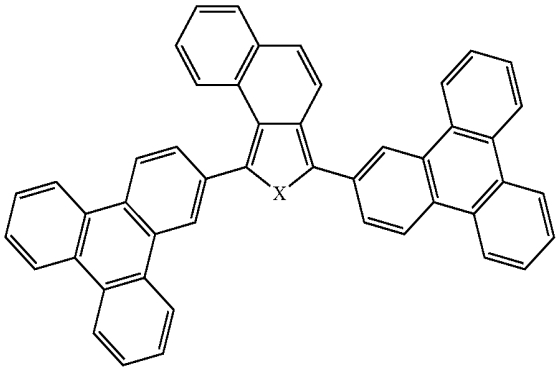
Compound 4



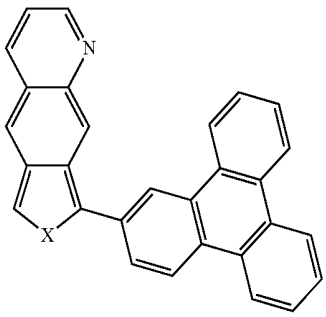
Compound 5



Compound 6



Compound 7



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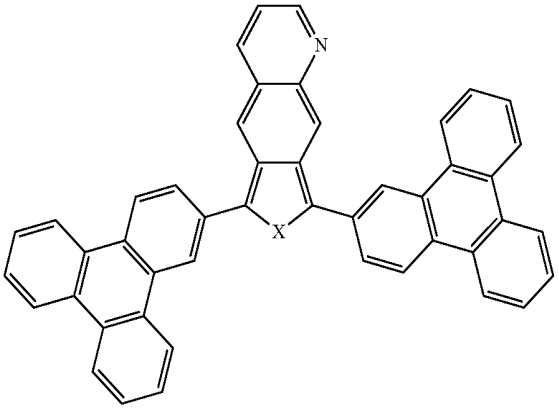
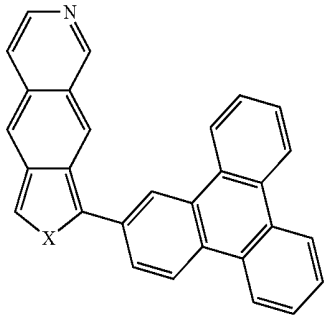
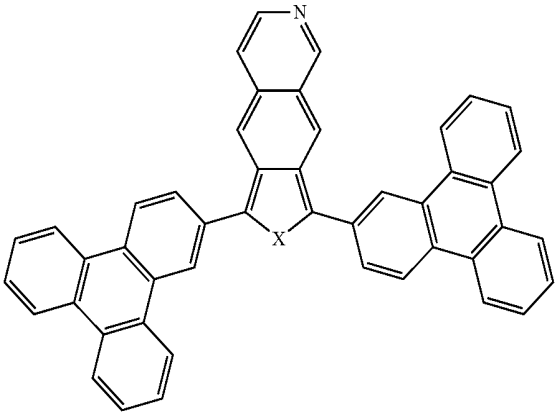
Compound 8



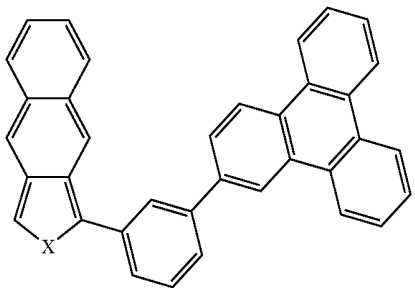
Compound 9



Compound 10



Compound 11



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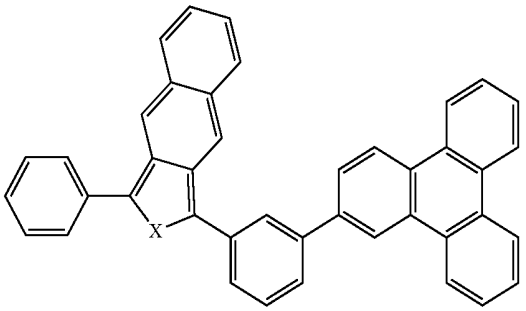
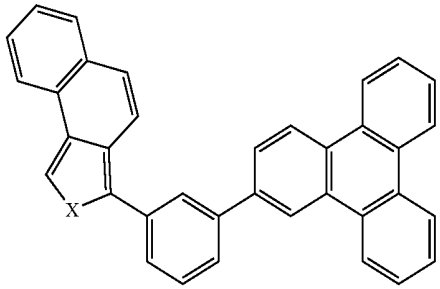
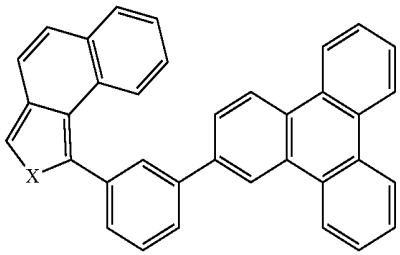
Compound 12



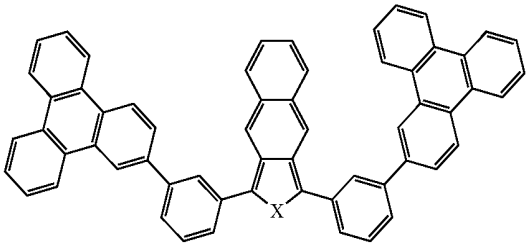
Compound 13



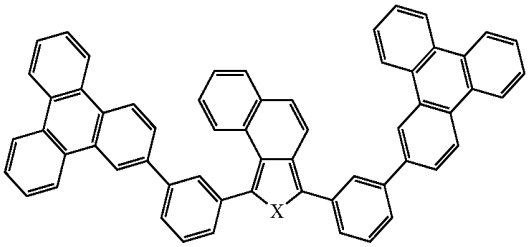
Compound 14



Compound15



Compound 16



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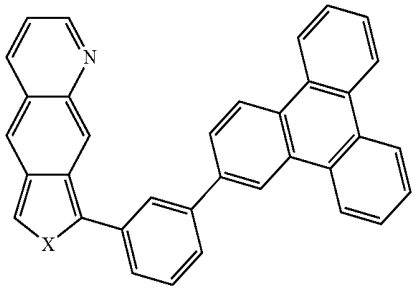
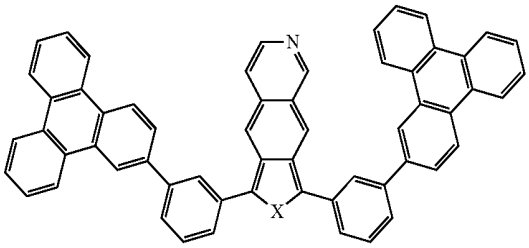
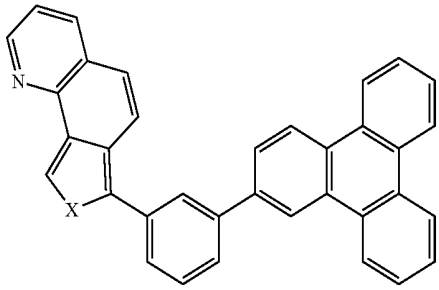
Compound 17



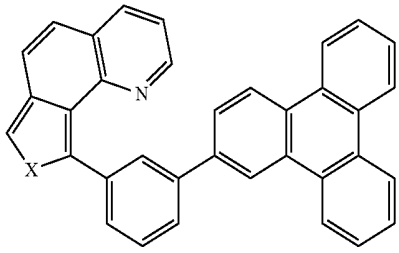
Compound 18



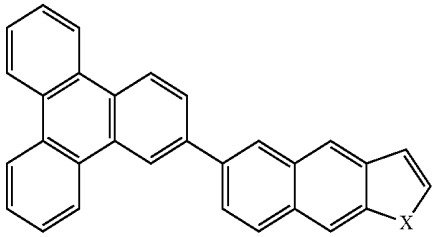
Compound 19



Compound 20



Compound 21



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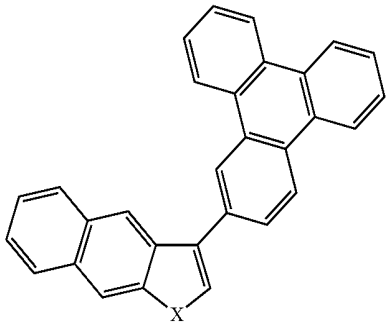
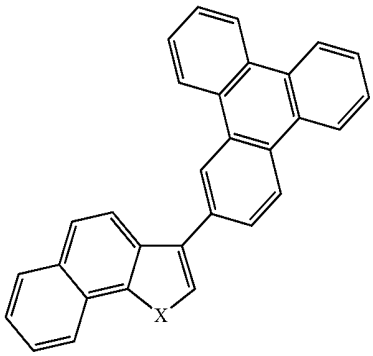
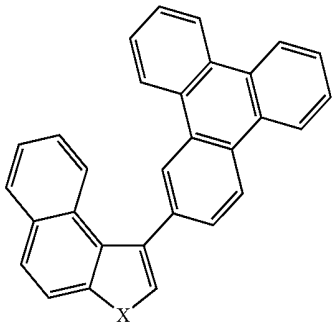
Compound 22



Compound 23



Compound 24



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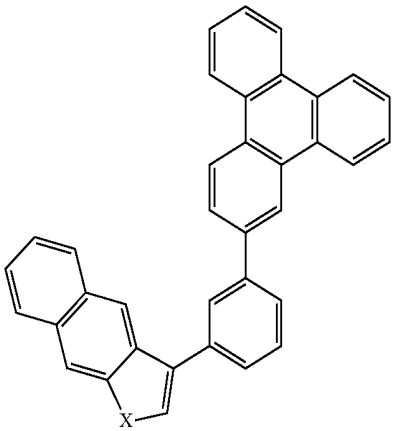

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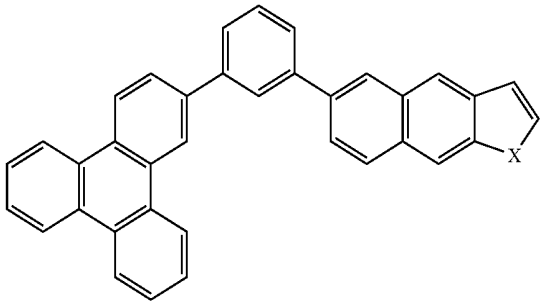
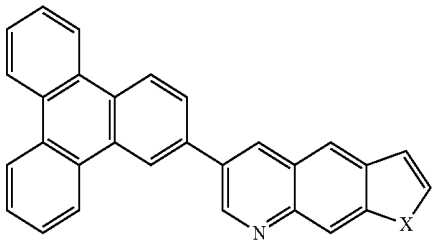
Compound 26



Compound 27



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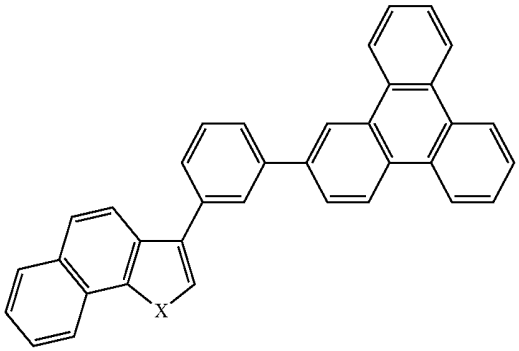

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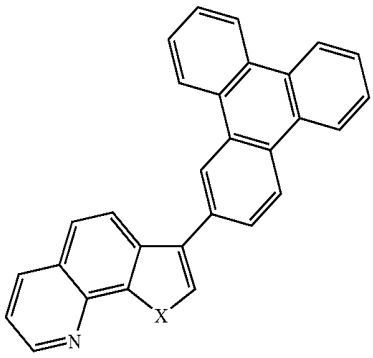

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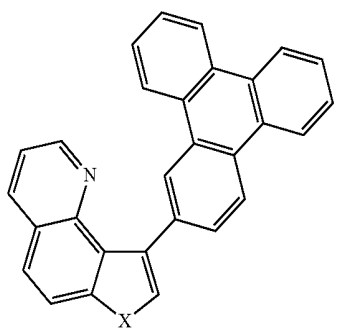

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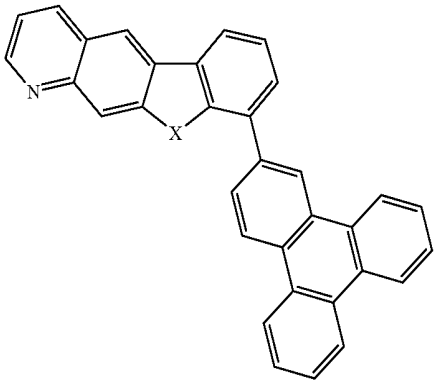
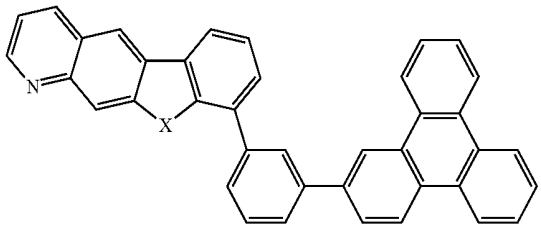
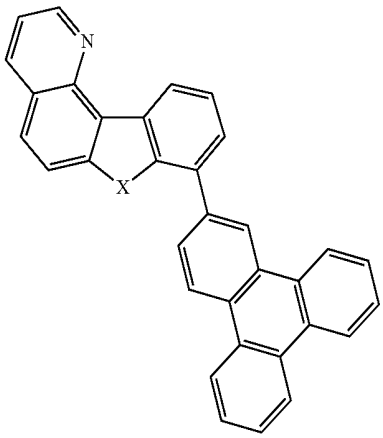
Compound 31



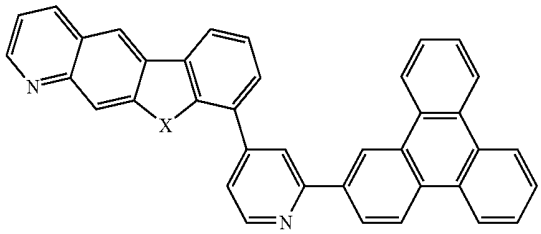
Compound 32



Compound 33



Compound 34



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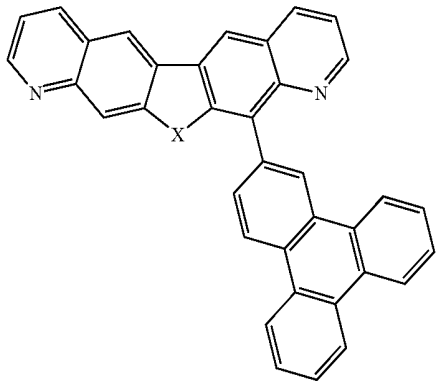
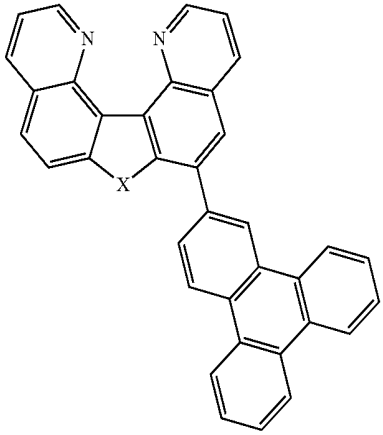
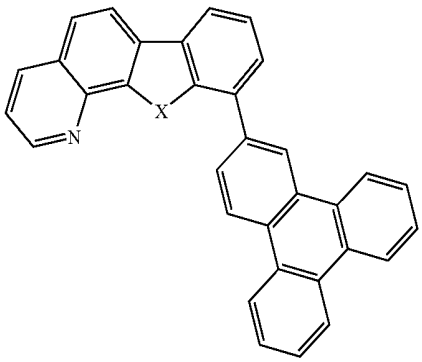
Compound 35



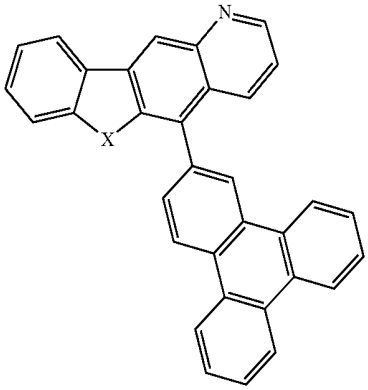
Compound 36



Compound 37



Compound 38



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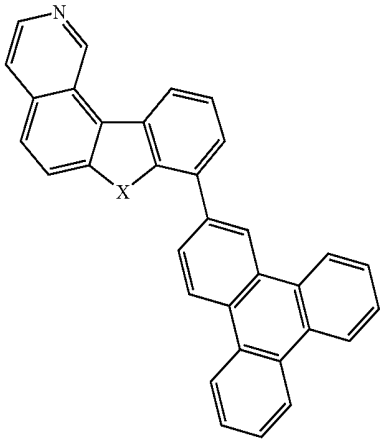
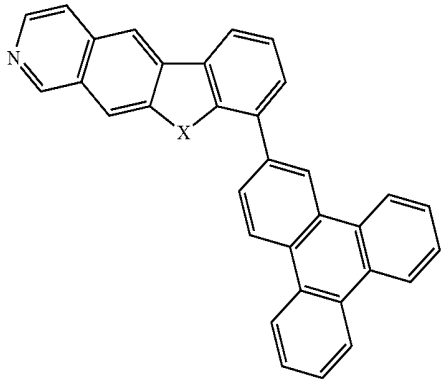
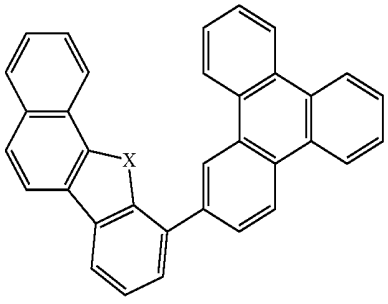
Compound 39



Compound 40



Compound 41



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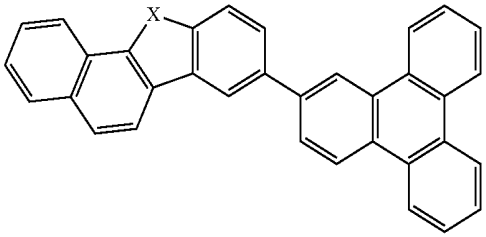

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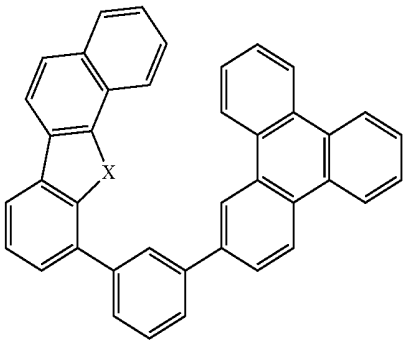
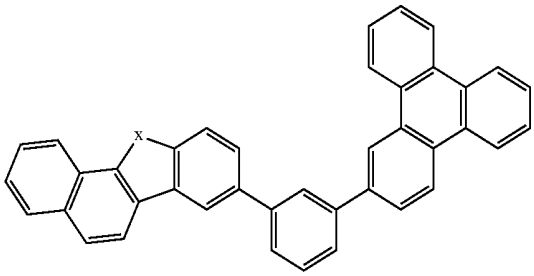
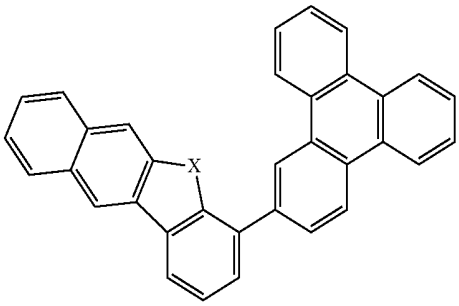
Compound 43



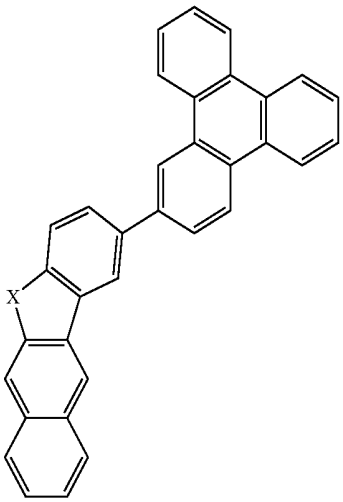
Compound 44



Compound 45



Compound 46



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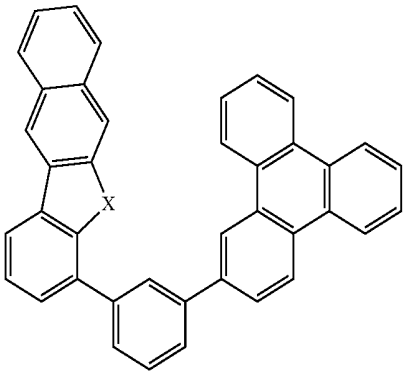
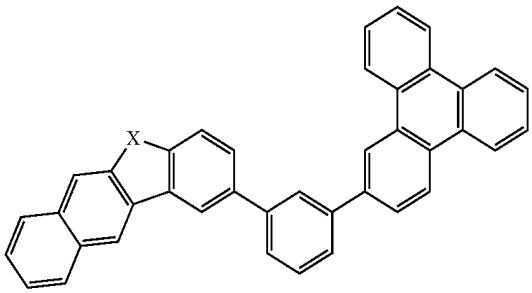
Compound 47



Compound 48



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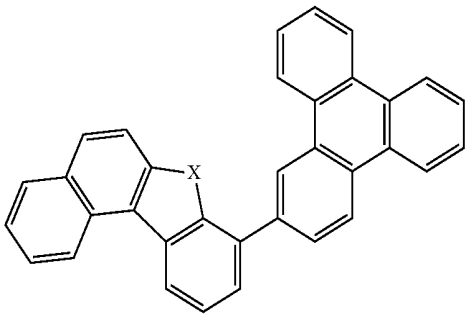
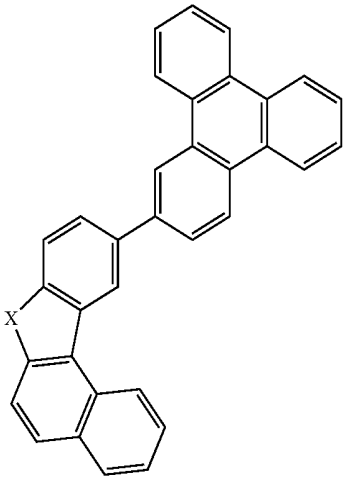


Compound 50



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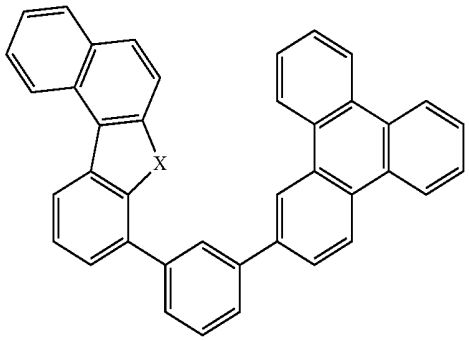
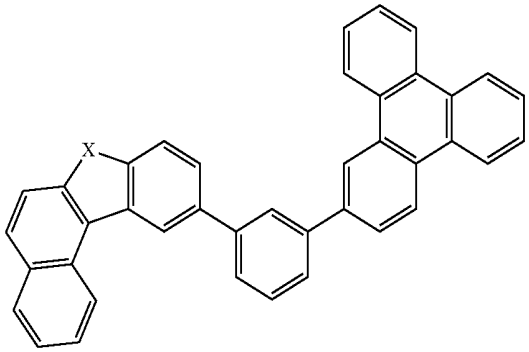
Compound 51



Compound 52



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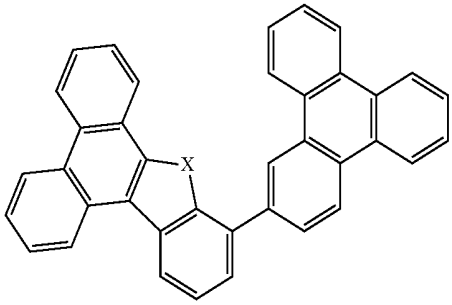
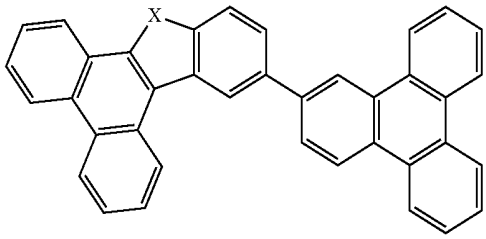


Compound 54



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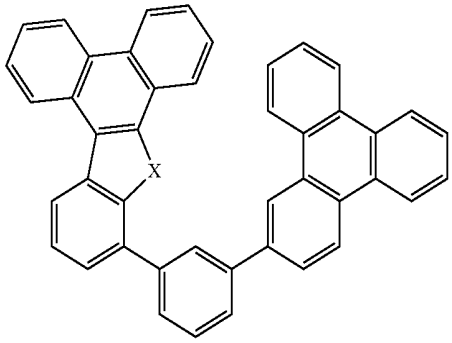

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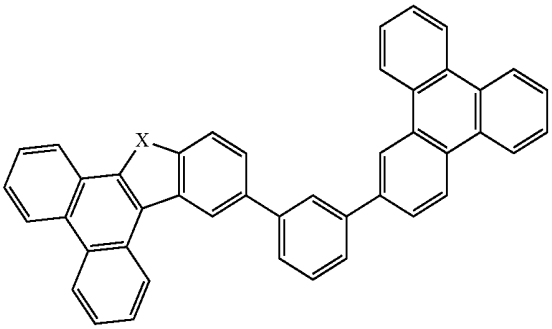
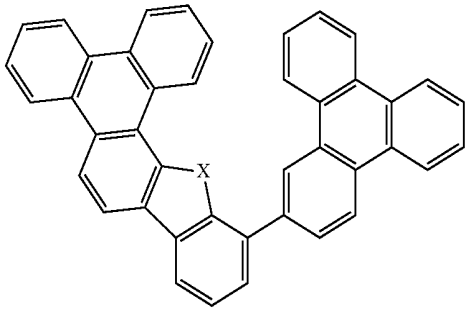
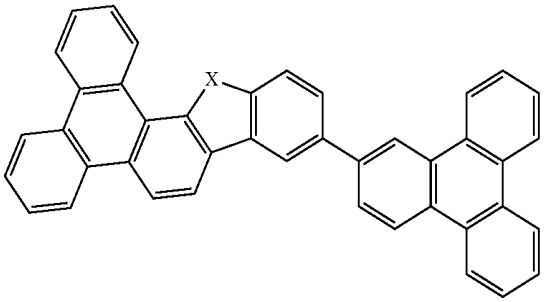
Compound 56



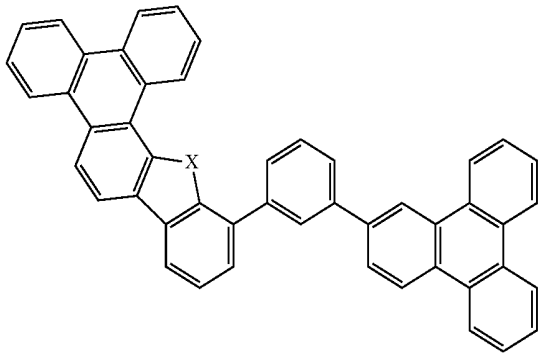
Compound 57



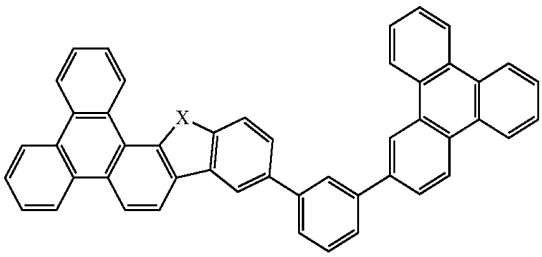
Compound 58



Compound 59



Coumpound 60



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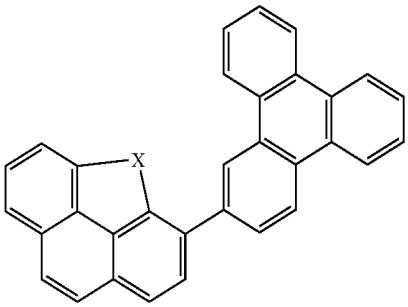
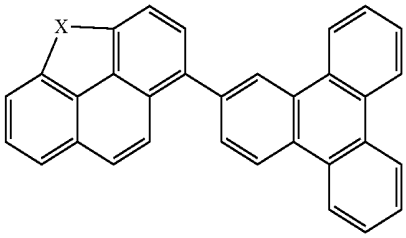
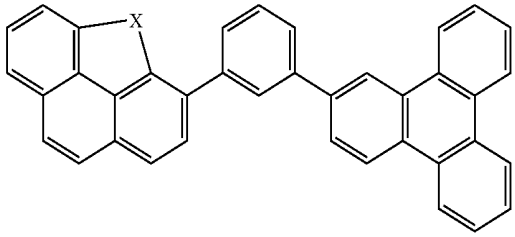
Compound 61



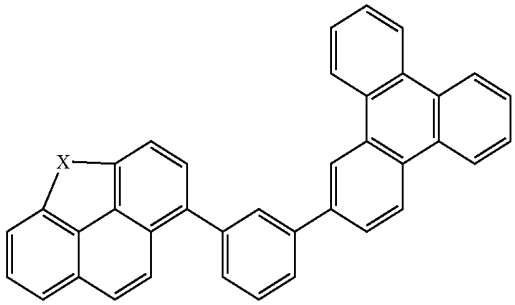
Compound 62



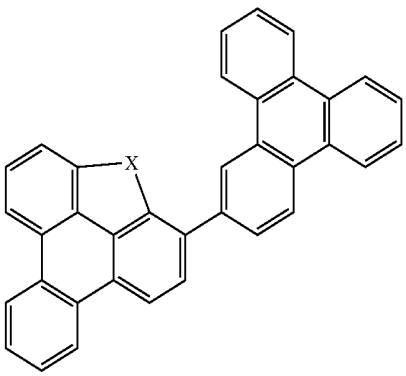
Compound 63



Compound 64



Compound 65



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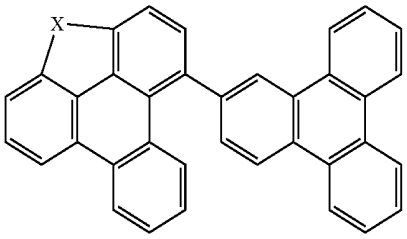
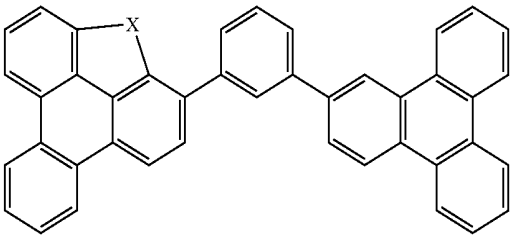
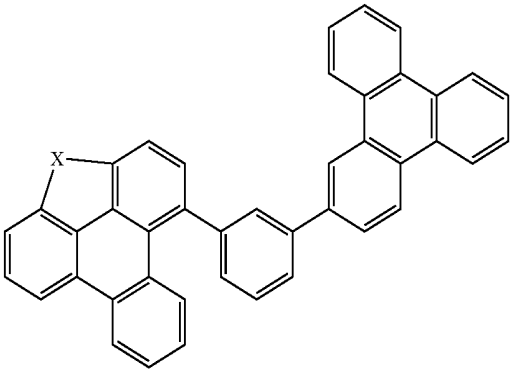
Compound 66



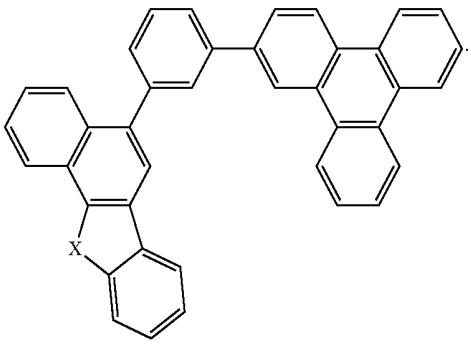
Compound 67



Compound 68



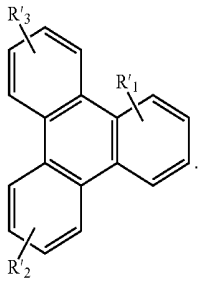
Compound 69



X is O, S, or Se.

Additionally, a first device comprising an organic light emitting device is provided. The organic light emitting device further comprises an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprises a compound comprising the formula:

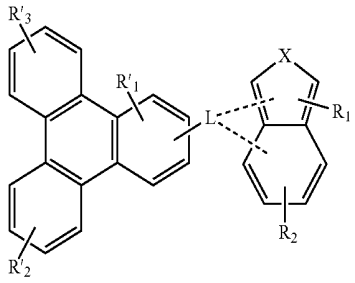
Formula I



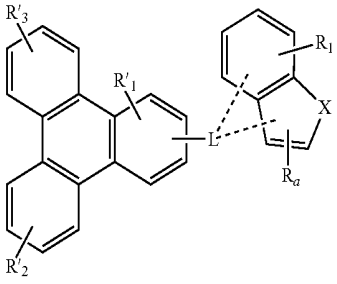
R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R'_1, R'_2, and R'_3 may represent mono, di, tri, or tetra substituents. The compound further comprises a benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety further comprising an additional aromatic or heteroaromatic ring fused to a benzo ring of the benzofuran, benzothiophene, benzoselenophene, dibenzofuran, dibenzothiophene, or dibenzoselenophene moiety.

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

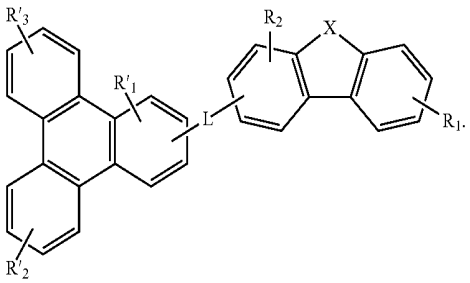
Formula 2



Formula 3



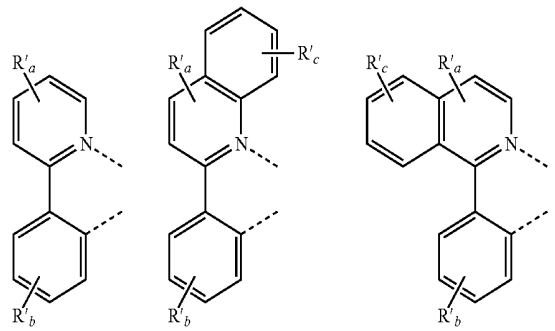
Formula 4

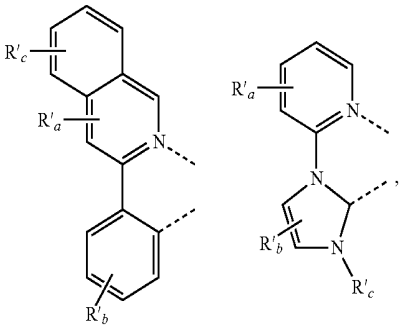


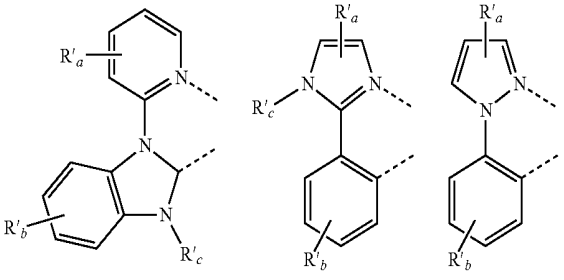
X is O, S or Se. R_1, R_2, and R_a are independently selected from hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Each of R_1 and R_2 may represent mono, di, tri or tetra substituents. At least two substituents of R_1 or R_2 are joined to form a fused ring. R_a

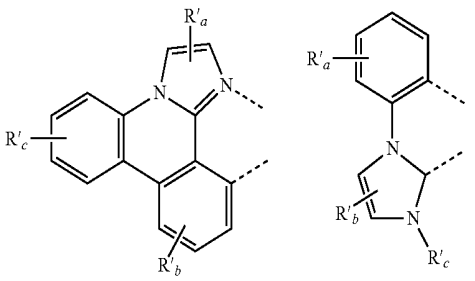
represents mono or di substituents which cannot fuse to form a benzo ring. L represents a spacer or a direct connection to the benzofuran, dibenzofuran, benzothiophene, dibenzothiophene, benzoselenophene or dibenzoselenophene moiety with additional fused rings.

In one aspect, the organic layer is an emissive layer and the compound comprising Formula I is the host. In another aspect, the organic layer further comprises an emissive compound. In yet another aspect, the emissive compound is a transition metal complex having at least one ligand selected from the group consisting of:









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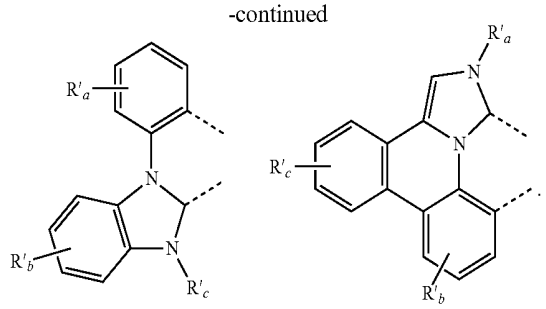


Each of R'_a, R'_b and R'_c may represent mono, di, tri, or tetra substituents. Each of R'_a, R'_b and R'_c are independently selected from a group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, or heteroaryl. Two adjacent substituents may form into a ring.

In another aspect, the device comprises a second organic layer that is non-emissive, and the compound comprising Formula I is a non-emissive material in the second organic layer.

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

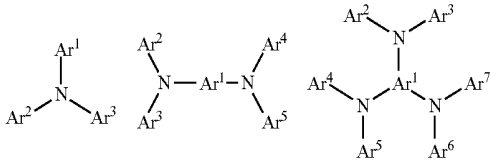
Combination with Other Materials

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

HIL/HTL:

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

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



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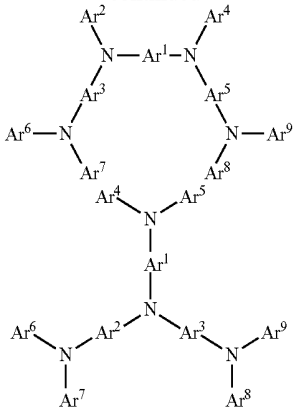
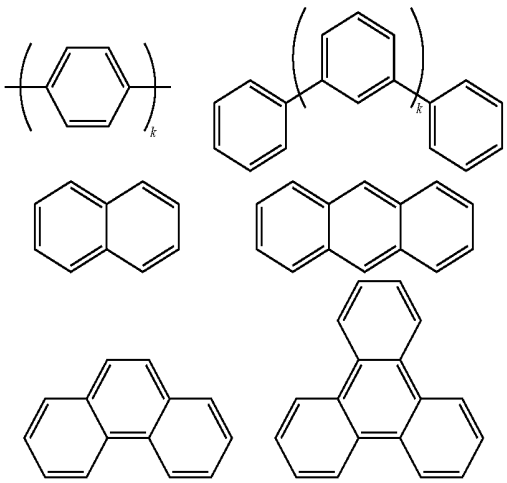


Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:



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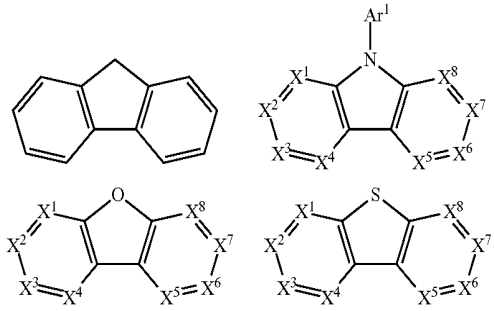
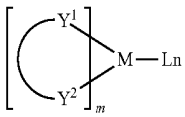


k is an integer from 1 to 20; X^1 to X^8 is CH or N; Ar^1 has the same group defined above.

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



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

In one aspect, $(Y^1\text{-}Y^2)$ is a 2-phenylpyridine derivative.

In another aspect, $(Y^1\text{-}Y^2)$ is a carbene ligand.

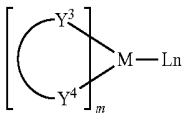
In another aspect, M is selected from Ir, Pt, Os, and Zn.

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

Host:

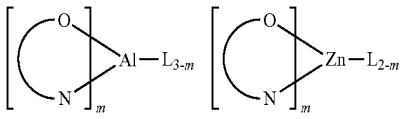
The light emitting layer of the organic EL device in some embodiments of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited,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

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



M is a metal; $(Y^3\text{-}Y^4)$ is a bidentate ligand, Y^3 and Y^4 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

In one aspect, the metal complexes are:



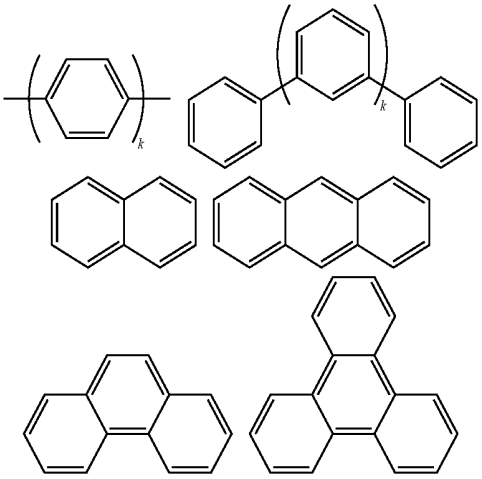
(O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

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

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

Examples of organic compounds used as hosts are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

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



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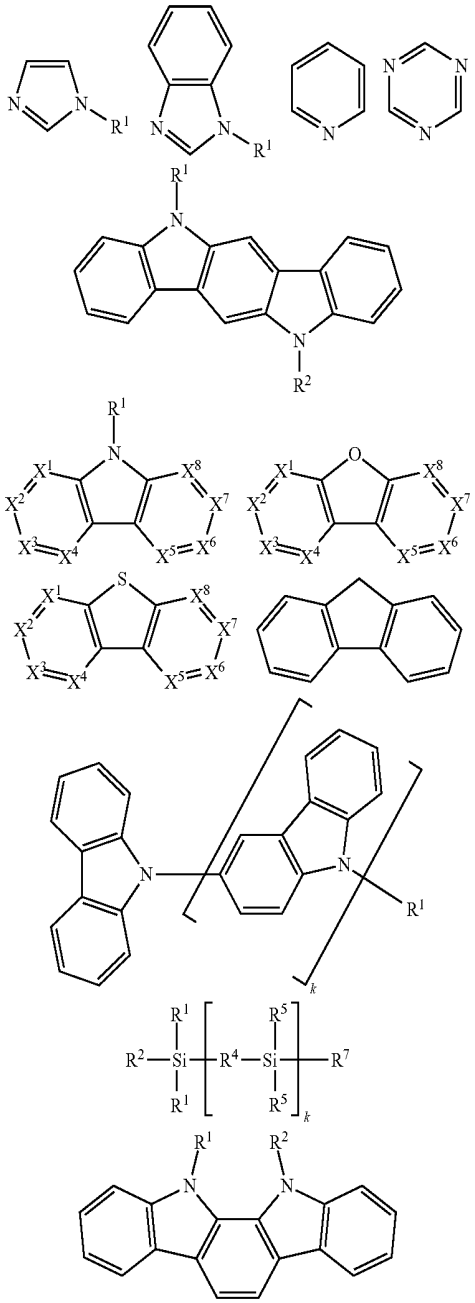


R^1 to R^7 is independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

k is an integer from 0 to 20.

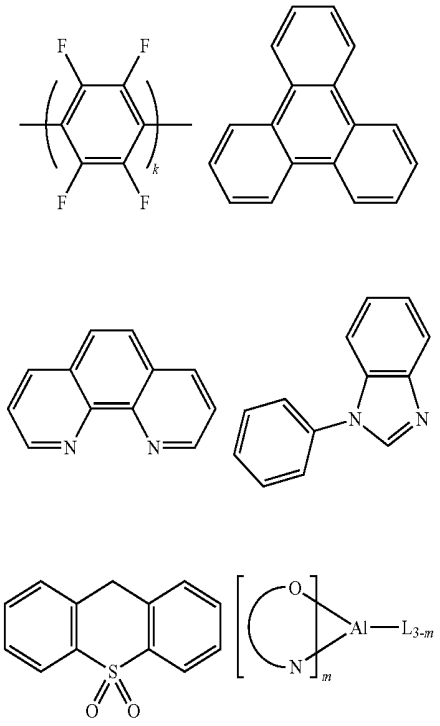
X^1 to X^8 is selected from CH or N.

HBL:

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

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

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

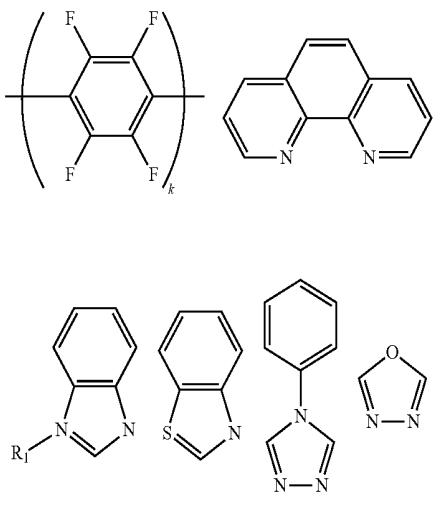


k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

ETL:

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

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



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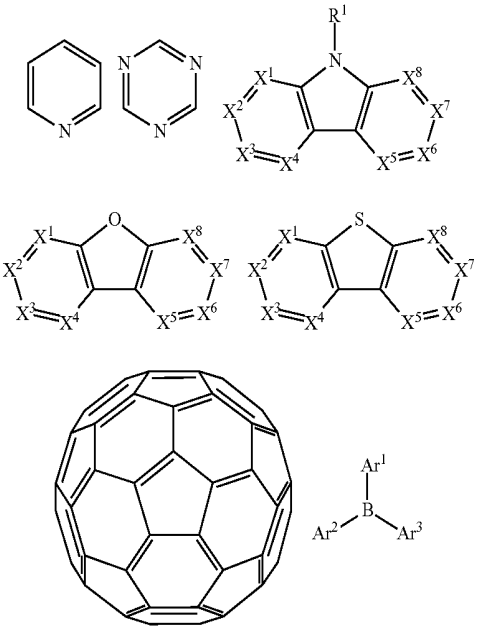


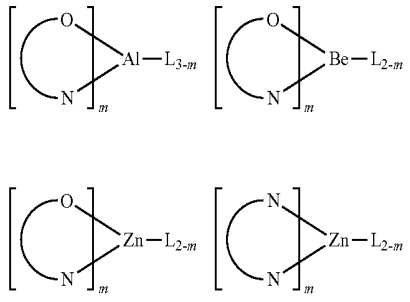
R^1 is selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

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

k is an integer from 0 to 20.

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

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



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

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

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

TABLE 1

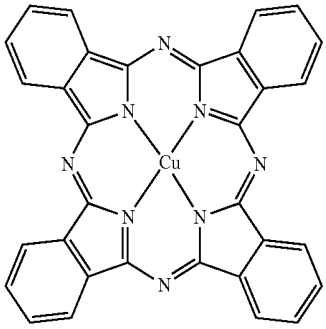
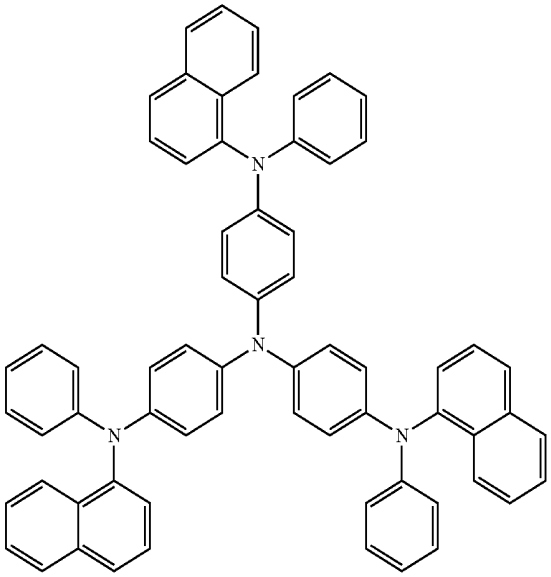
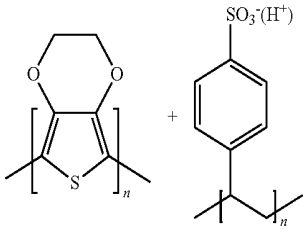
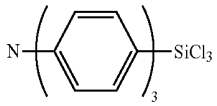
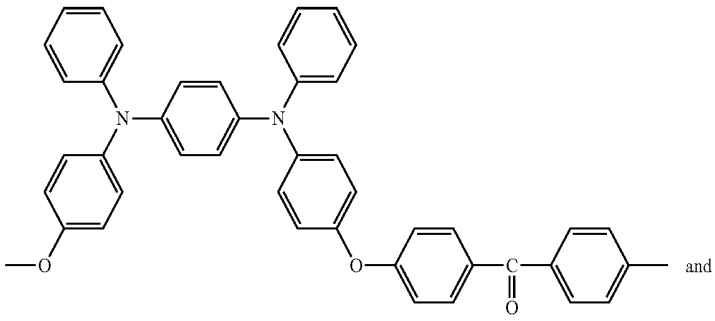
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphyrin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydrocarbon polymer		Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and sliane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants	 and	EA01725079A1

TABLE 1-continued

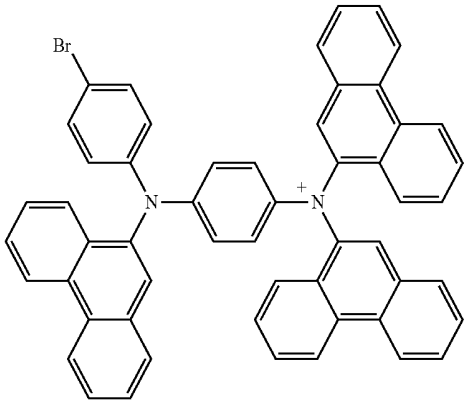
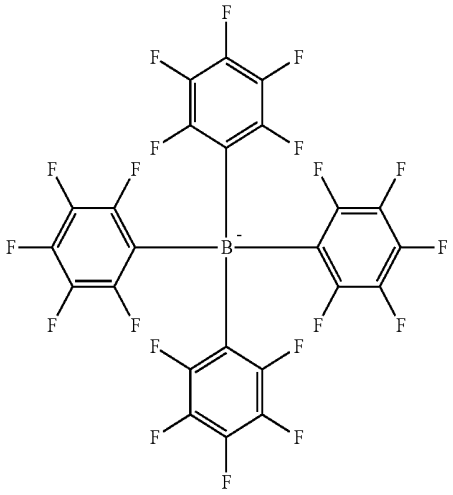
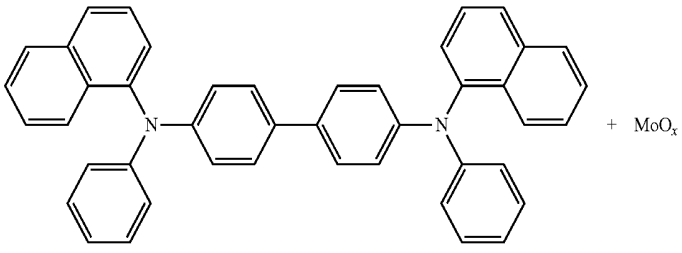
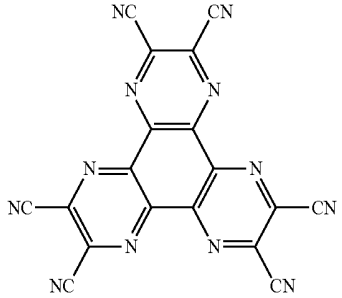
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		
		
Arylamines complexed with metal oxides such as molybdenum and tungsten oxides		SID Symposium Digest, 37, 923 (2006) WO2009018009
p-type semiconducting organic complexes		US20020158242

TABLE 1-continued

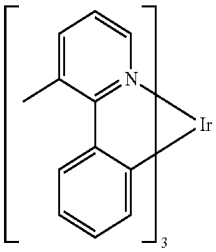
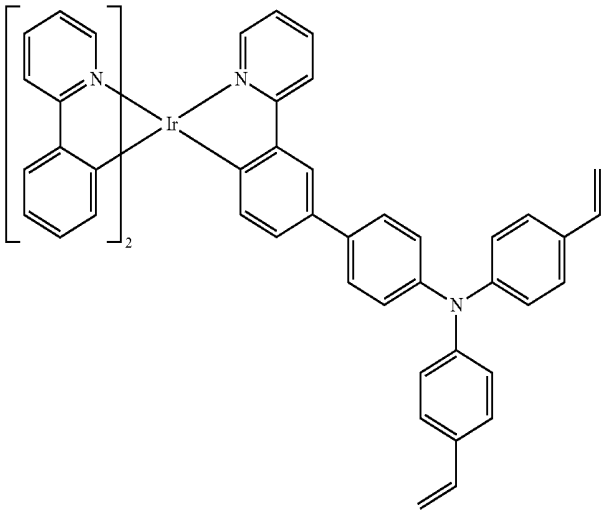
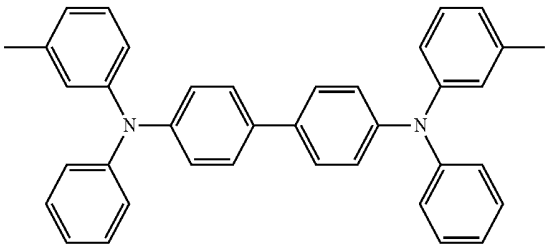
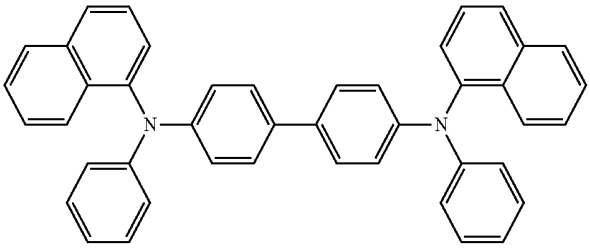
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal organo-metallic com-plexes		US20060240279
Cross-linkable compounds		US20080220265
Hole transporting materials		
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		US5061569

TABLE 1-continued

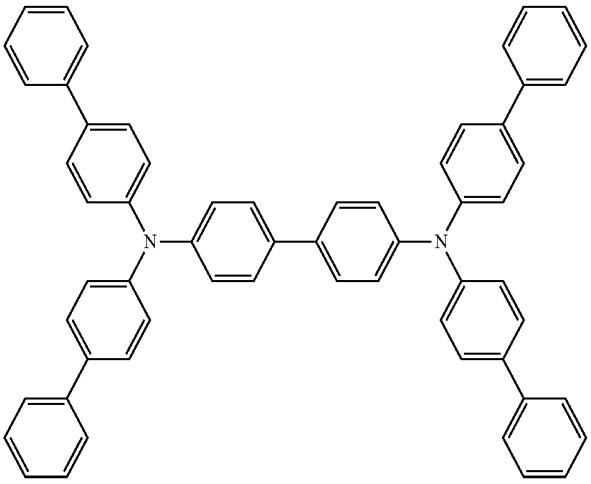
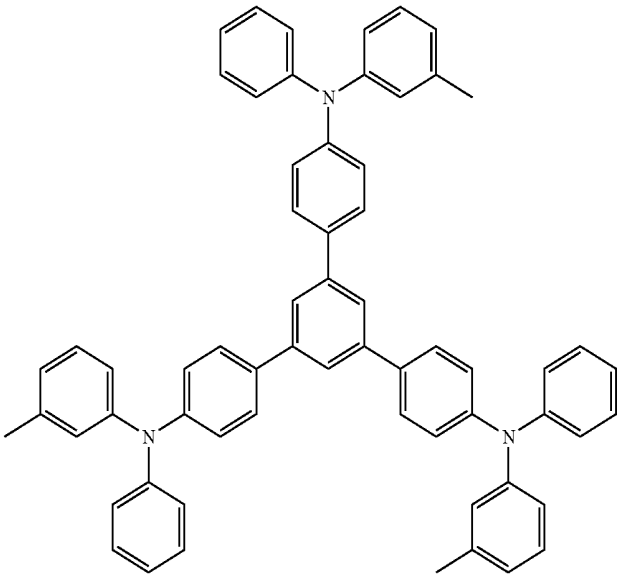
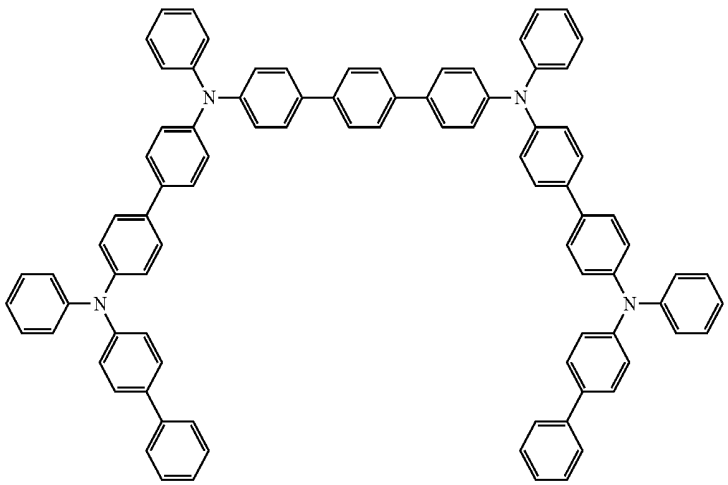
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		EP650955
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE 1-continued

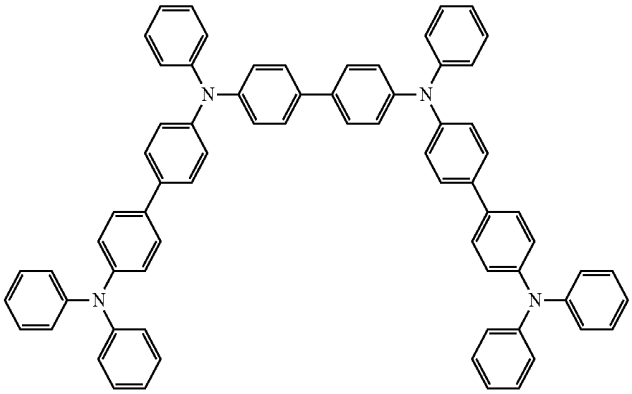
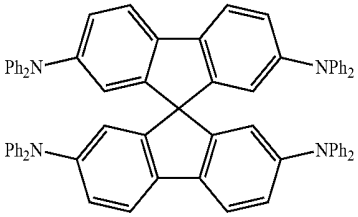
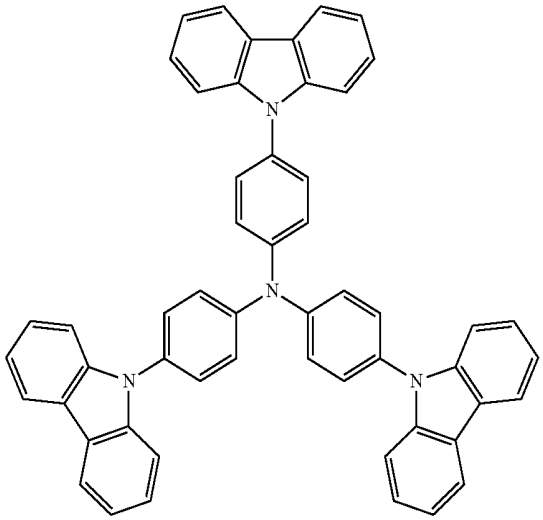
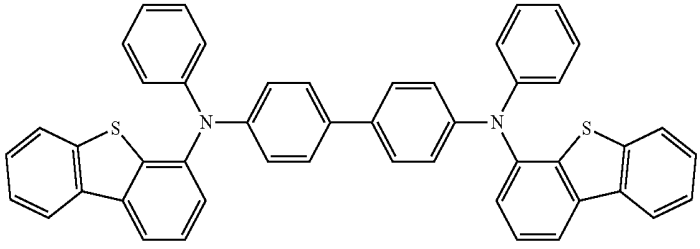
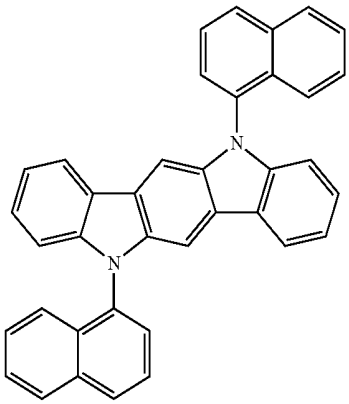
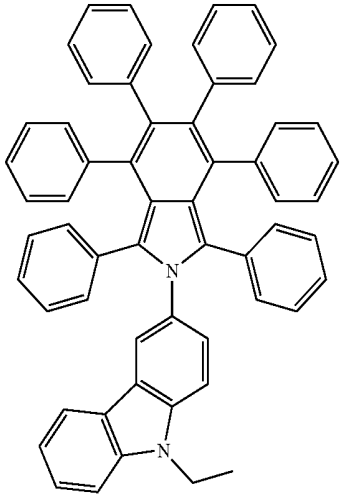
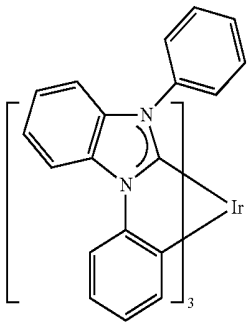
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
Triarylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/(di)benzofuran		US20070278938, US20080106190

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocar-bazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221

Phosphorescent OLED host materials

Red hosts

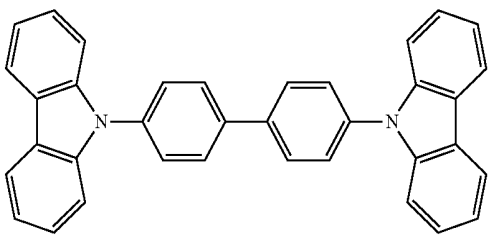
Arylcar-bazoles		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

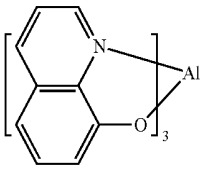
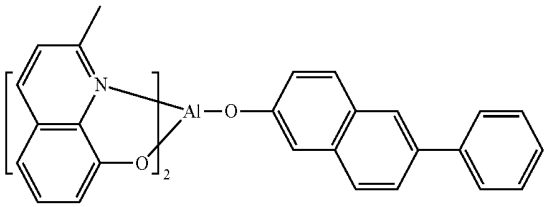
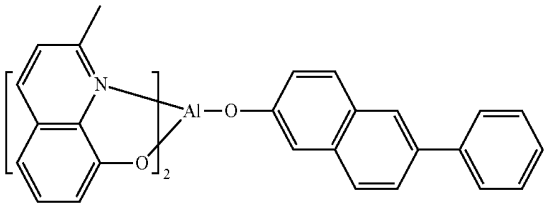
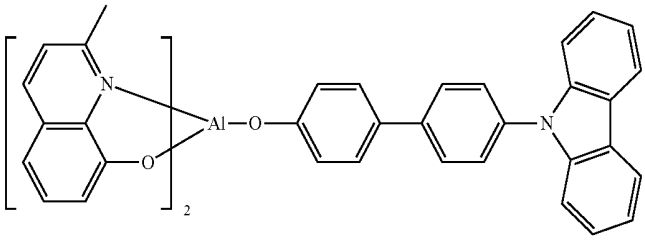
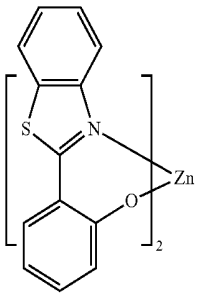
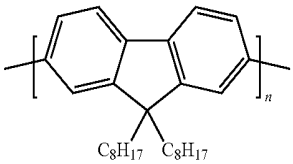
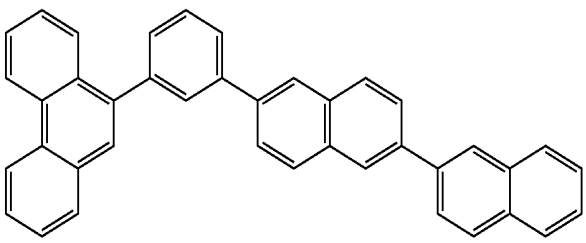
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065

TABLE 1-continued

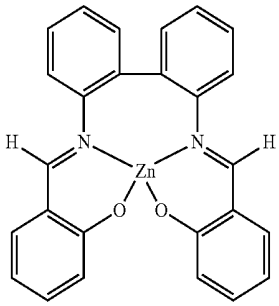
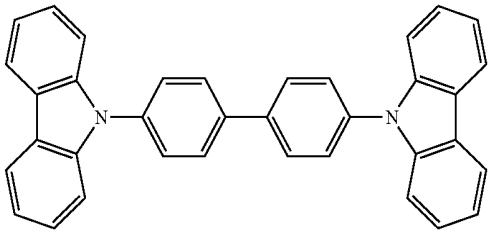
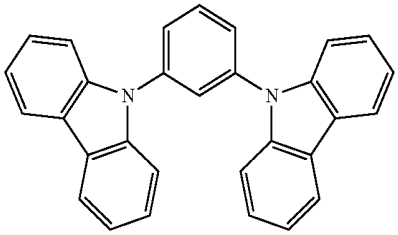
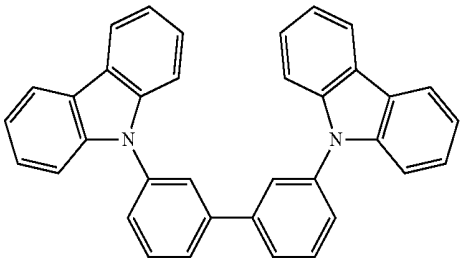
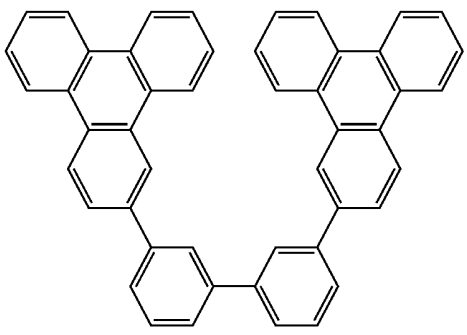
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Zinc complexes		WO2009062578
	Green hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE 1-continued

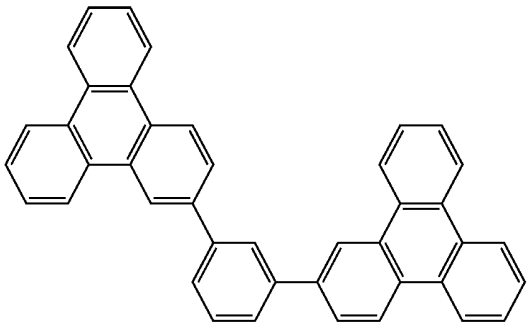
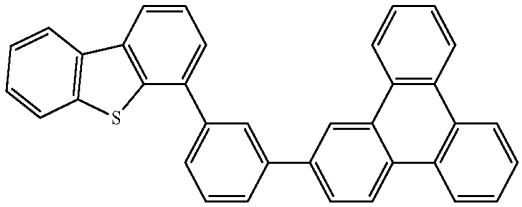
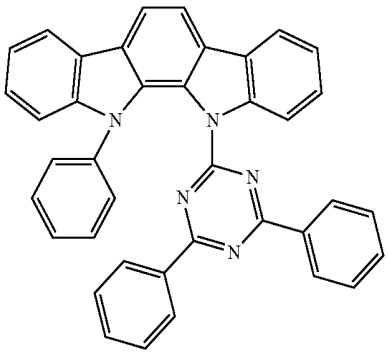
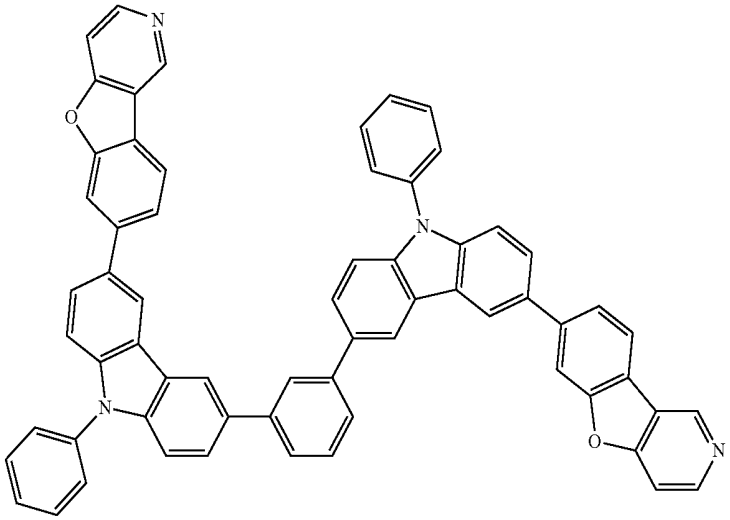
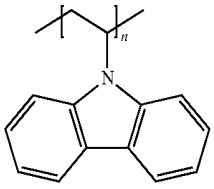
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060280965
		WP2009021126
Donor acceptor type molecules		WO2008056746
Aza-carbazole/ DBT/DBF		JP2008074939
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)

TABLE 1-continued

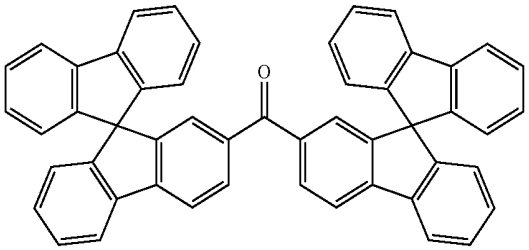
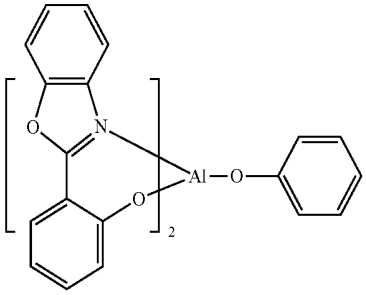
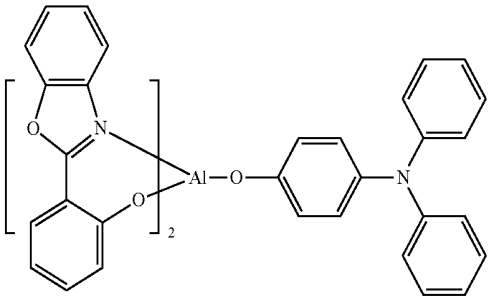
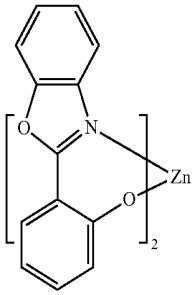
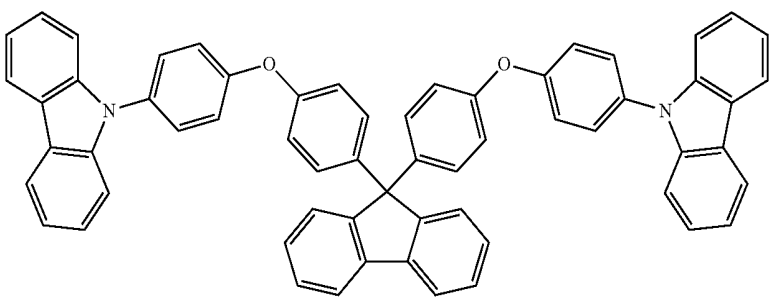
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Spirofluorene compounds		WO2004093207
Metal phenoxybenzooxazole compounds		WO2005089025
		WO20066132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297

TABLE 1-continued

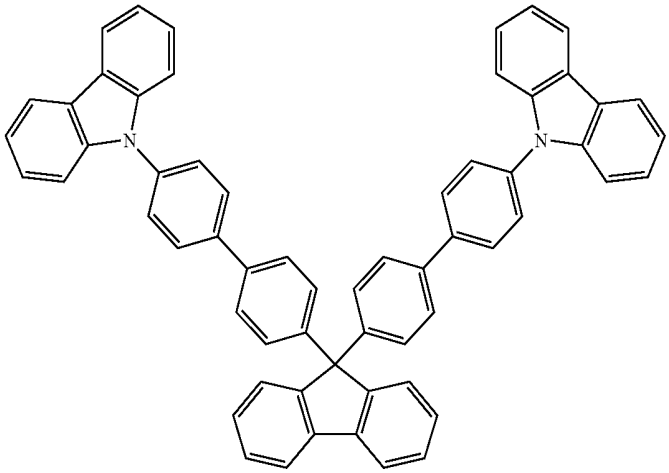
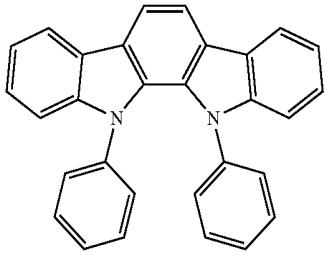
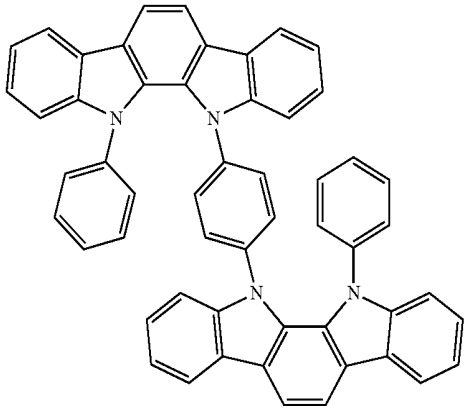
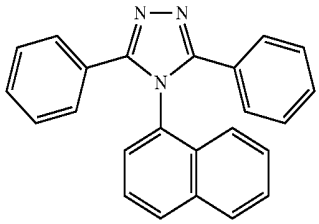
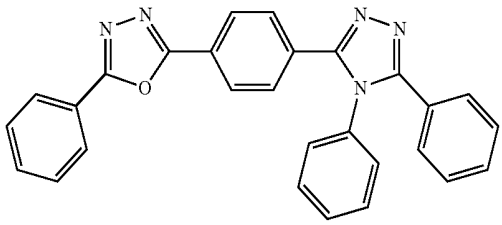
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		JP2007254297
Indolo-cabazoles		WO2007063796
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822

TABLE 1-continued

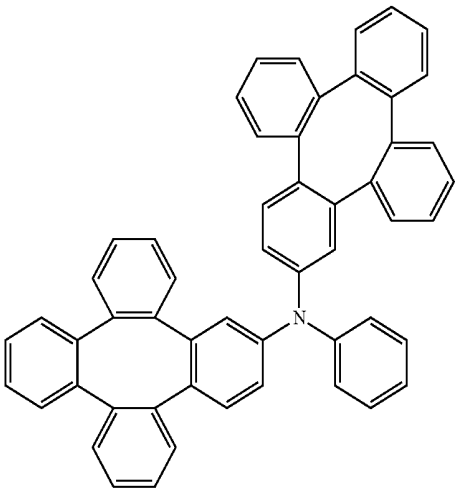
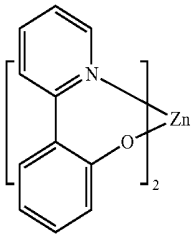
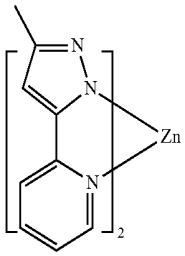
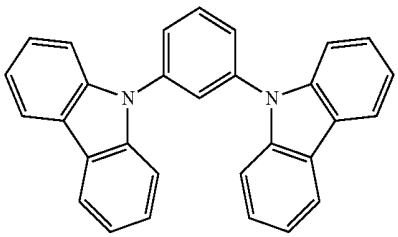
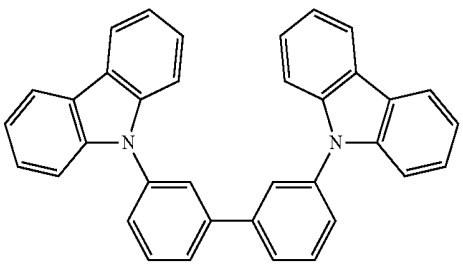
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al, with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359

TABLE 1-continued

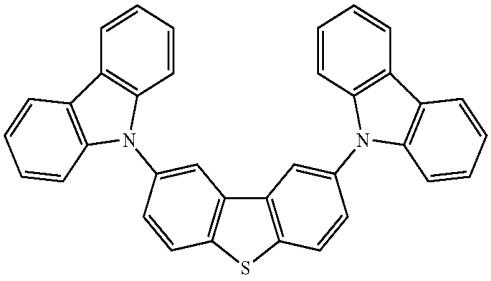
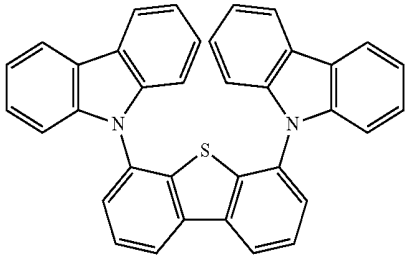
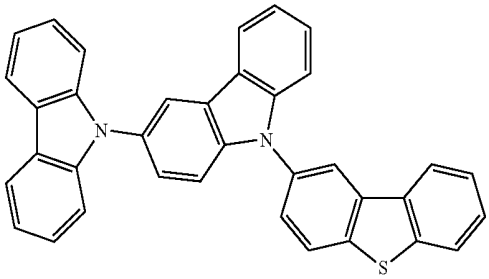
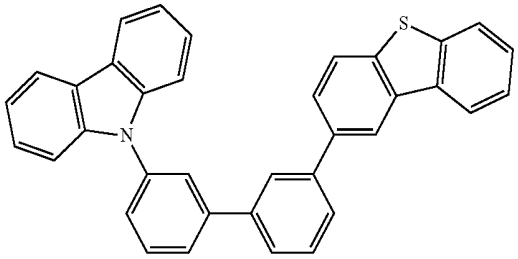
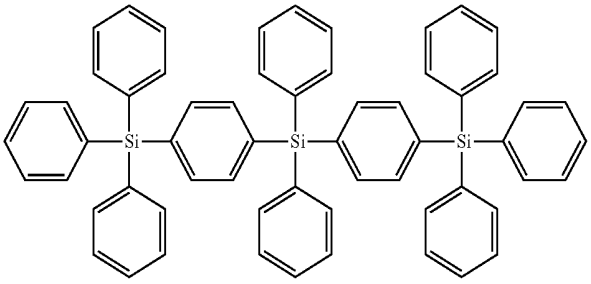
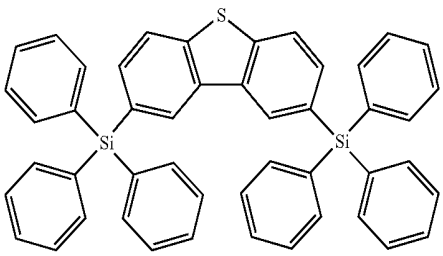
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzo-thiophene/ Diben-zofuran-carbazole compounds		WO20066114966, US20090167162
		US20090167162
		WO2009086028
		US20090030202, US20090017330
Silicon aryl compounds		US20050238919
		WO2009003898

TABLE 1-continued

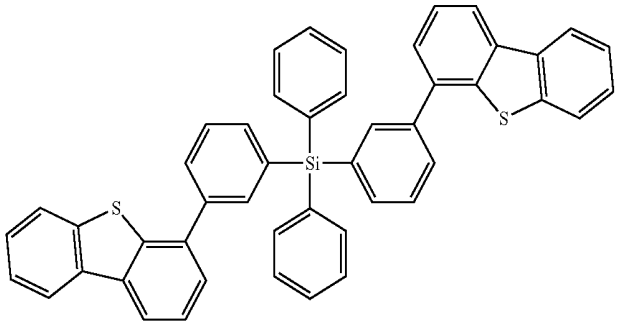
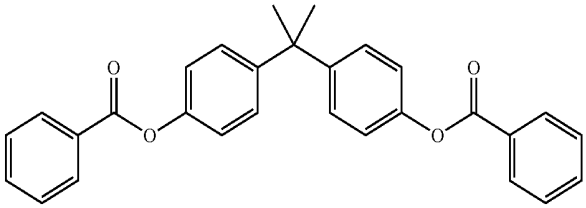
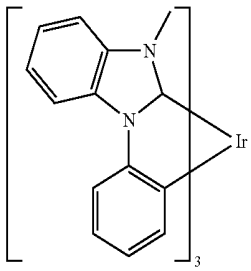
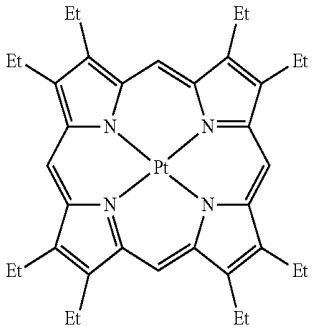
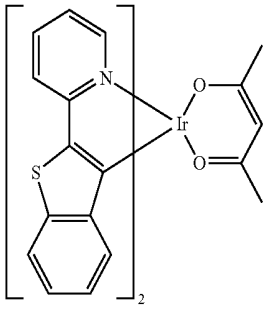
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon/ Germanium aryl compounds		WP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex		US7154114
Phosphorescent dopants		
Red dopants		
Heavy metal prophyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

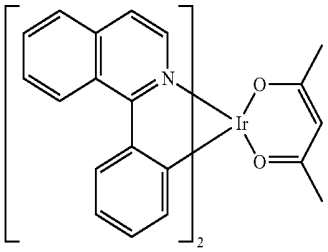
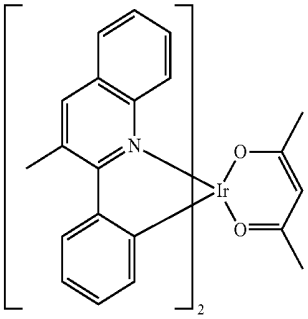
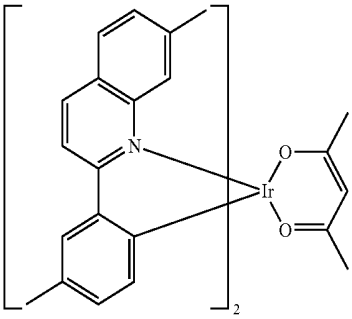
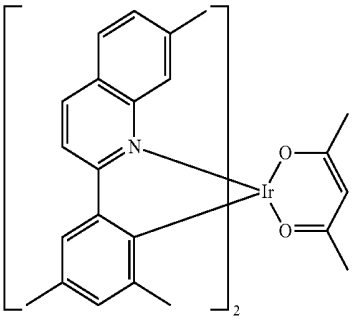
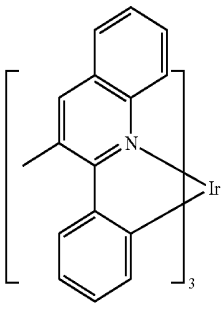
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US2006835469
		US2006835469
		US20060202194
		US20060202194
		US20070087321

TABLE 1-continued

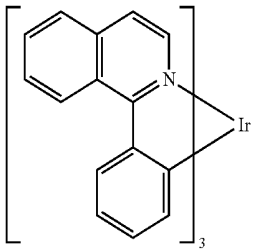
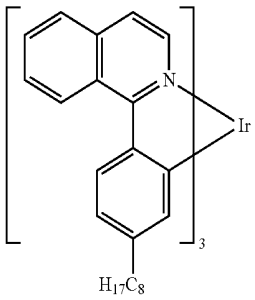
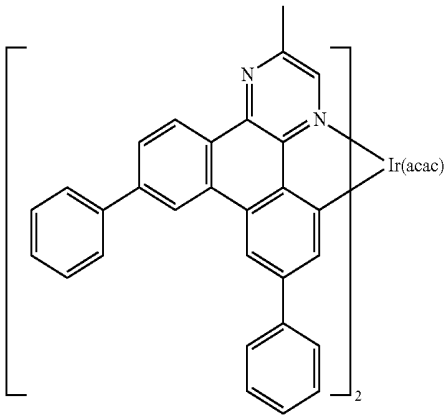
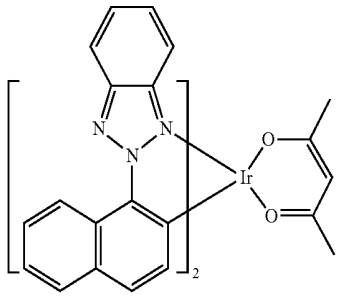
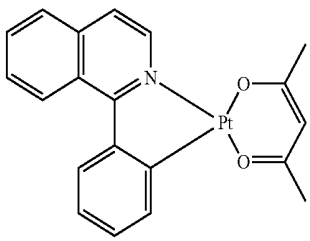
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
Platinum(II) organo-metallic complexes		WO2003040257

TABLE 1-continued

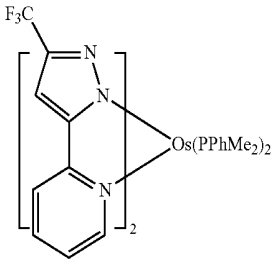
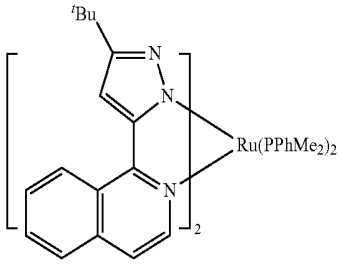
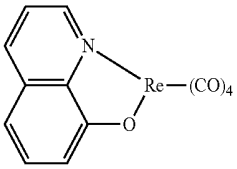
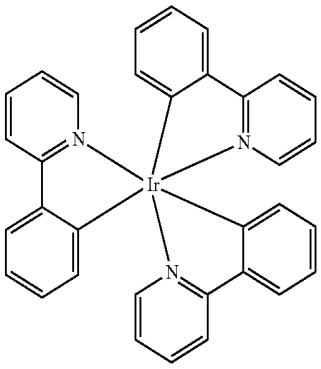
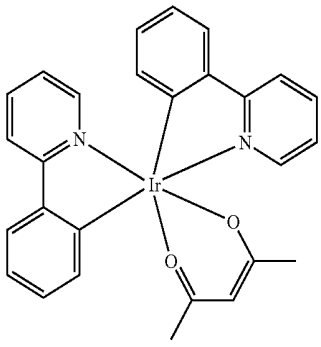
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruth-enium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
	Green dopants	
Iridium(III) organo-metallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656

TABLE 1-continued

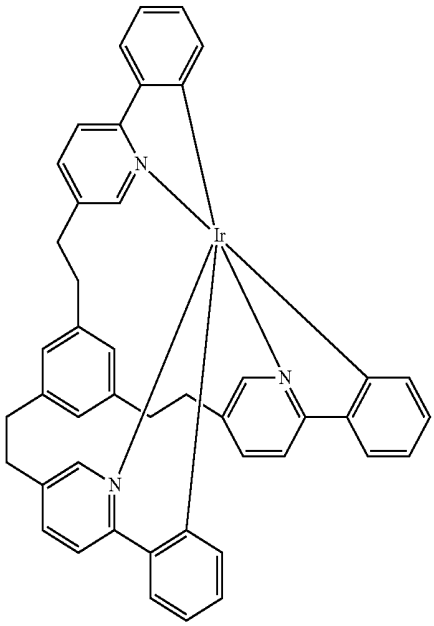
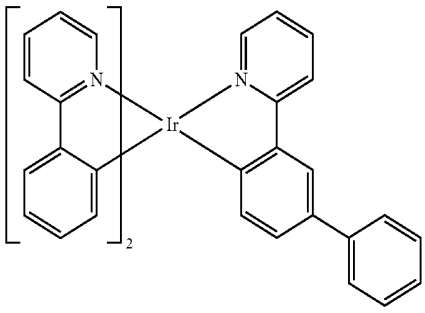
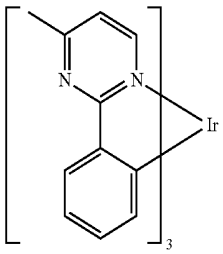
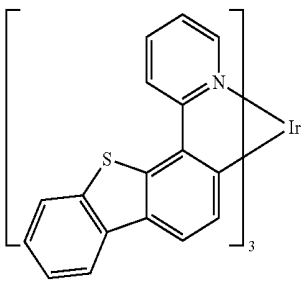
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7332232
		US20090108737
		US20090039776
		US6921915

TABLE 1-continued

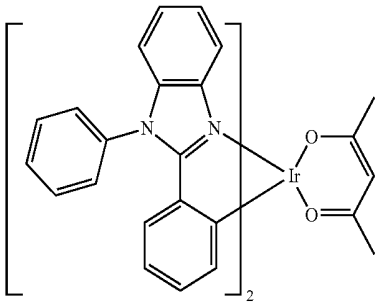
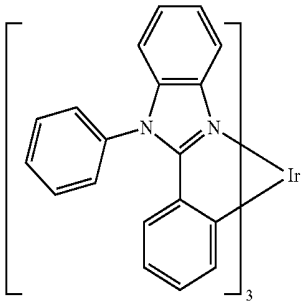
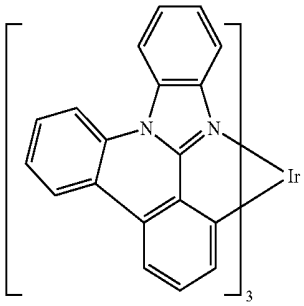
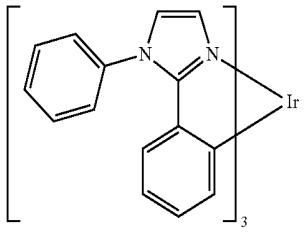
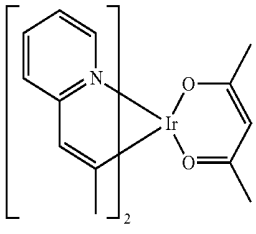
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US6687266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US20060008670 JP2007123392
		Adv. Mater. 16, 2003 (2004)

TABLE 1-continued

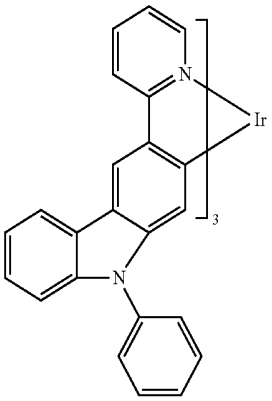
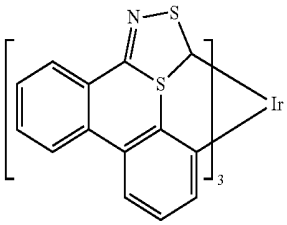
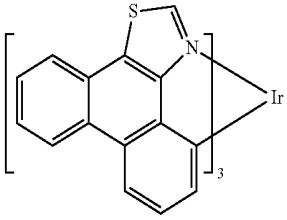
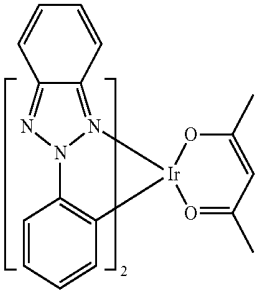
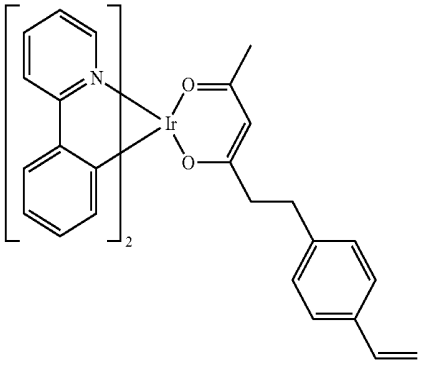
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846
		US20080015355
Monomer for polymeric metal organometallic compounds		US7250226, US7396598

TABLE 1-continued

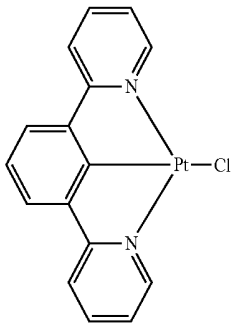
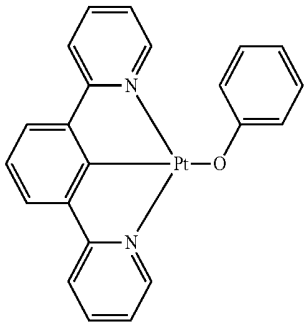
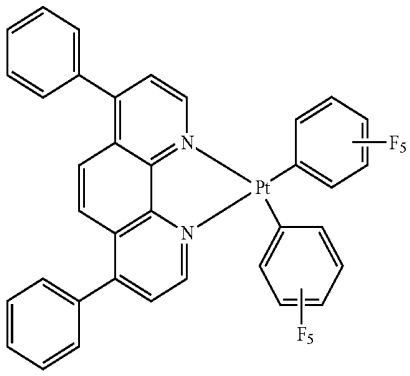
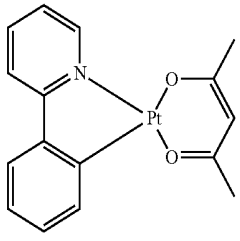
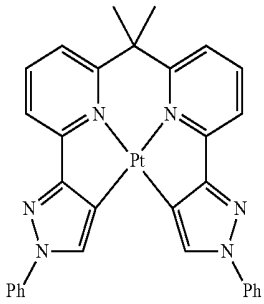
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635

TABLE 1-continued

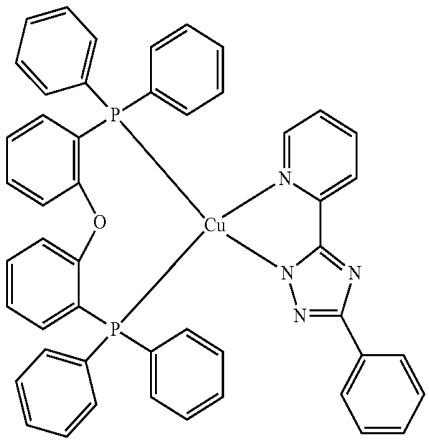
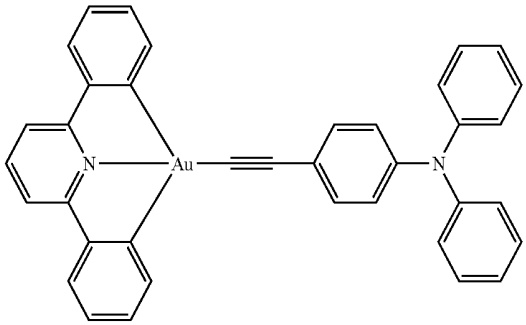
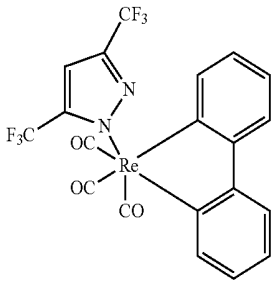
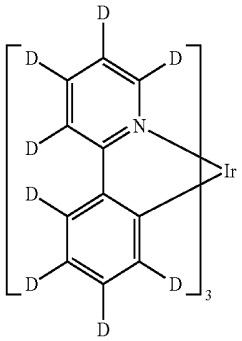
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)
Deuterated organometallic complexes		US20030138657

TABLE 1-continued

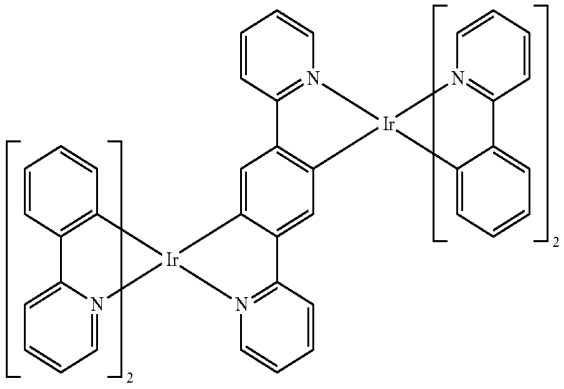
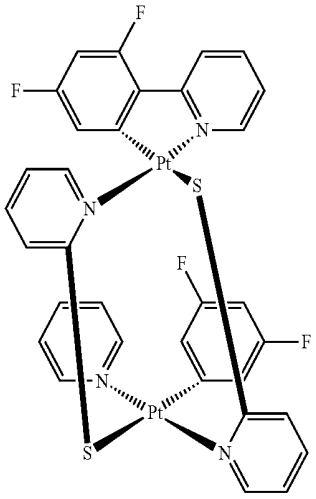
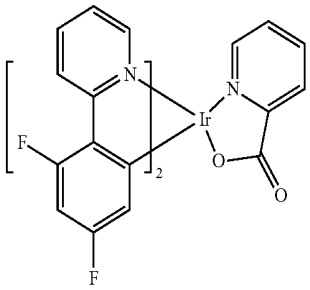
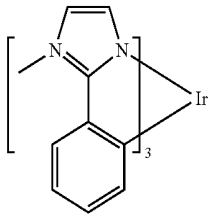
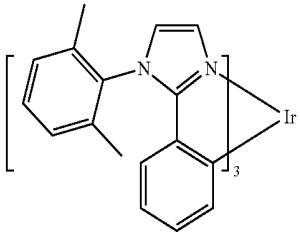
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organometallic complexes with two or more metal centers		US20030152802
		US7090928
Blue dopants		
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923

TABLE 1-continued

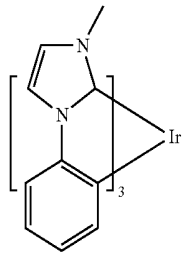
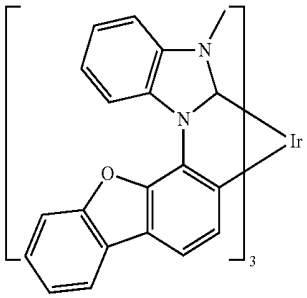
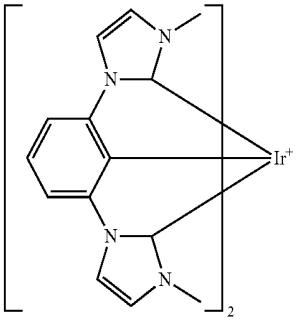
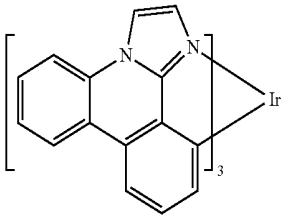
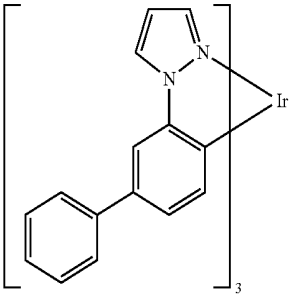
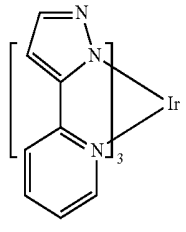
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7393599, WO2006056418, US20050260441, WO2005019373
		US7534505
		US7445855
		US20070190359, US20080297033
		US7338722
		US20020134984

TABLE 1-continued

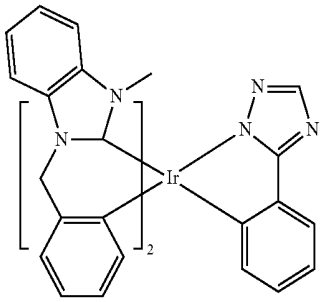
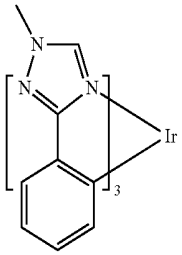
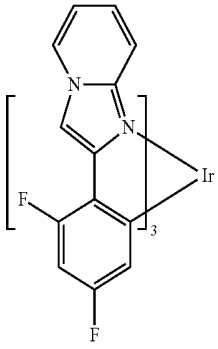
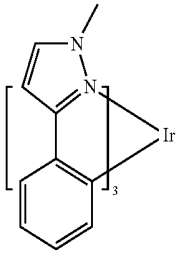
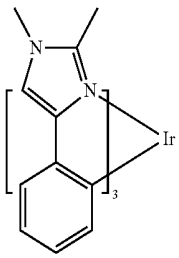
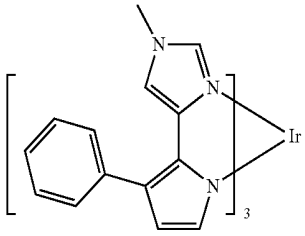
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380

TABLE 1-continued

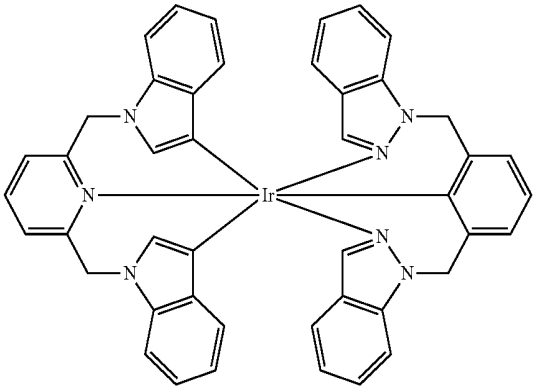
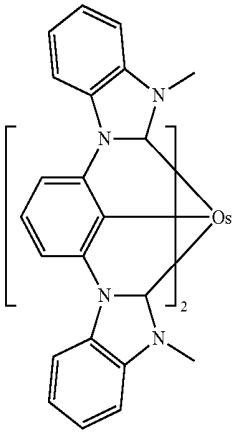
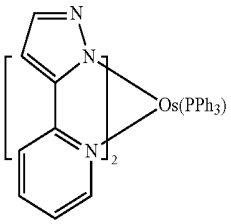
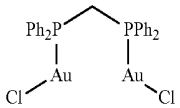
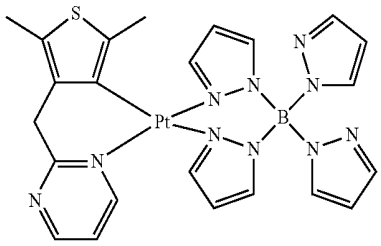
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006082742
Osmium(II) complexes		US7279704
		Organo-metallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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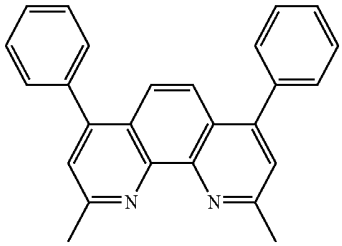
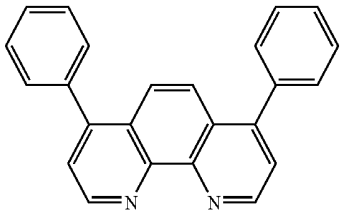
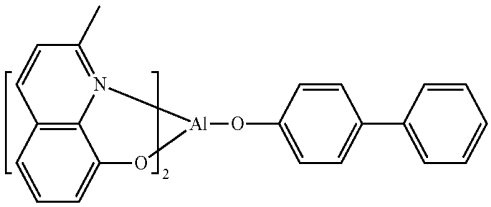
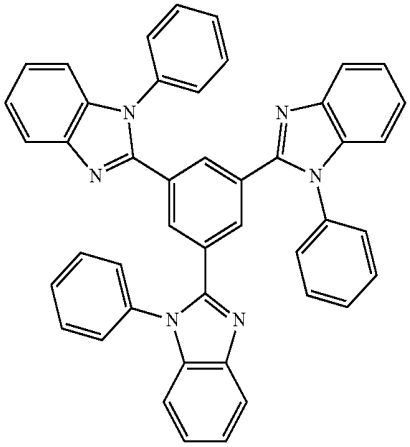
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)

TABLE 1-continued

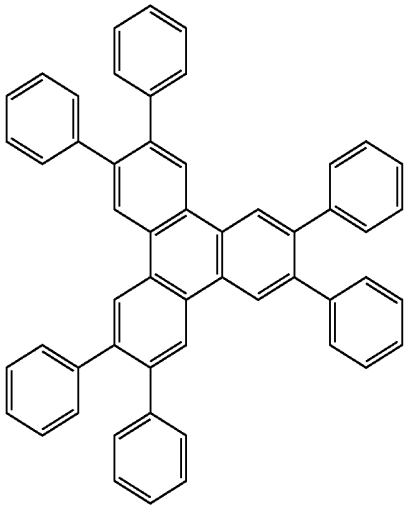
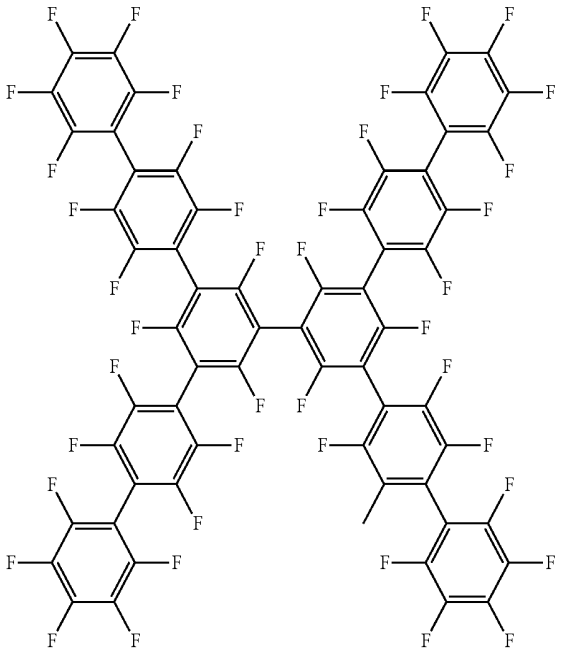
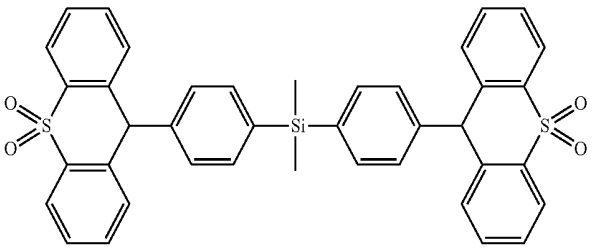
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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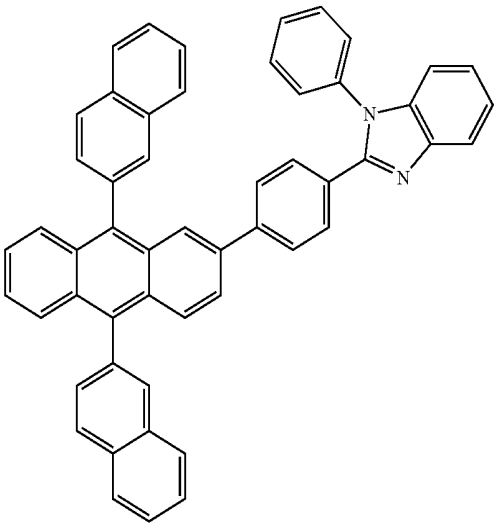
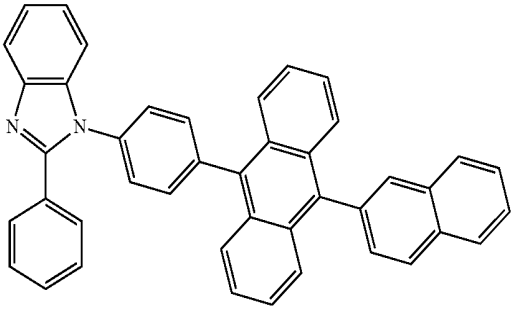
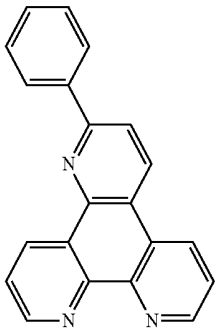
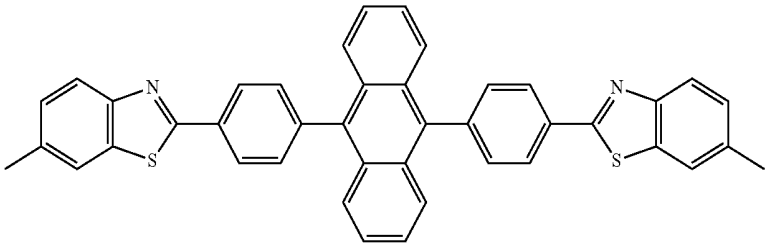
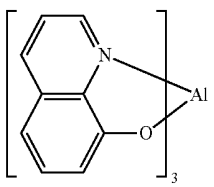
Anthracene-benzomidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) US7230107

TABLE 1-continued

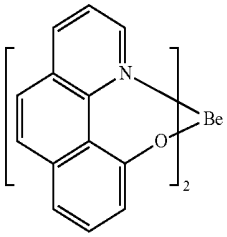
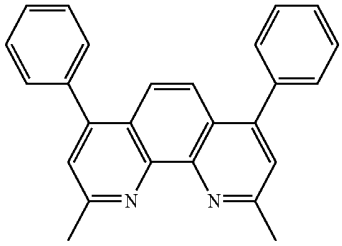
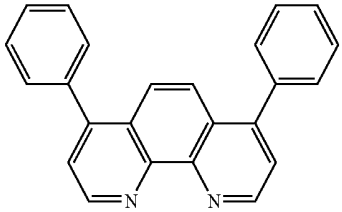
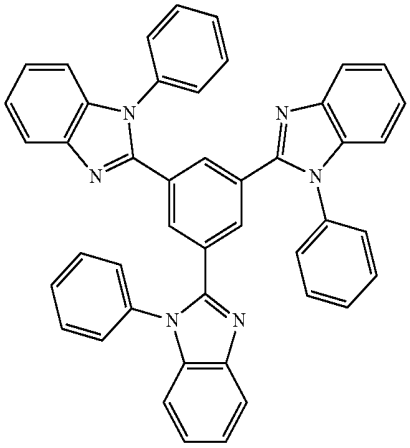
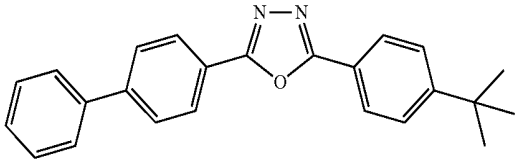
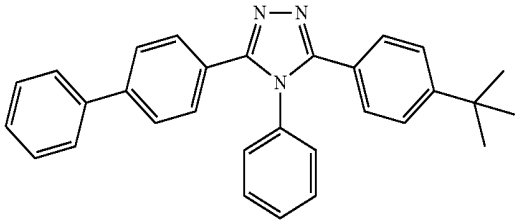
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal hydroxy-benoquin-olates		Chem. Lett. 5, 905 (1993)
Batho-cuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
		Appl. Phys. Lett. 79, 449 (2001)
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole,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

TABLE 1-continued

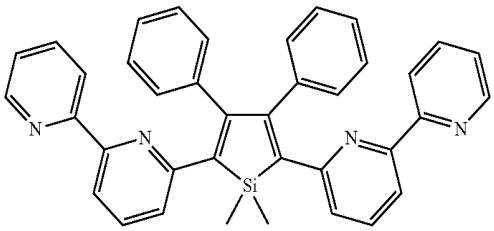
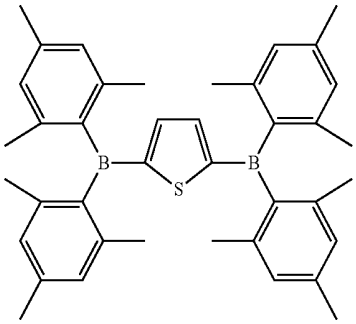
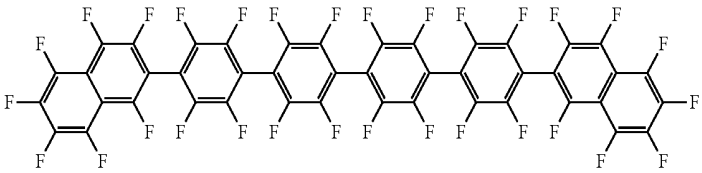
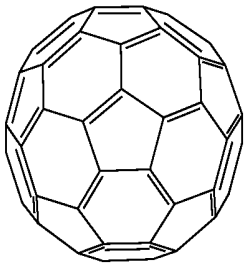
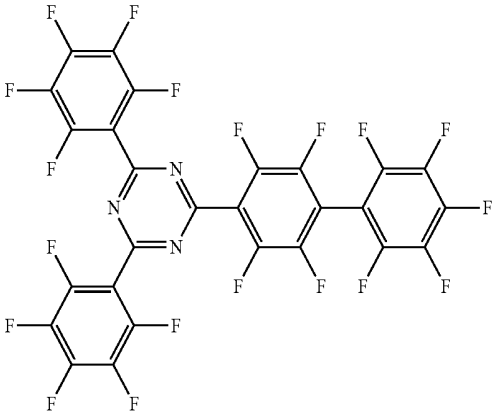
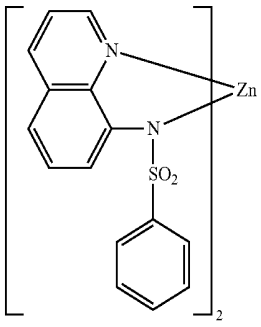
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silole compounds		Org. Electron. 4, 113 (2003)
Aryl-borane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluor-inated aro-matic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870
Triazine complexes		US20040036077

TABLE 1-continued

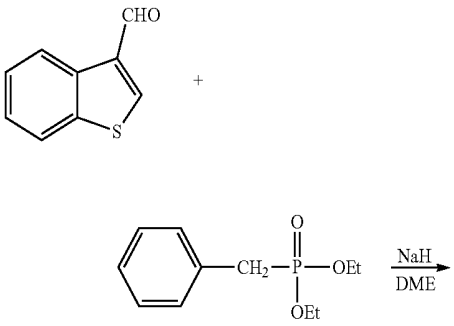
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Zn (N^N) complexes		US6528187

EXPERIMENTAL

Compound Examples

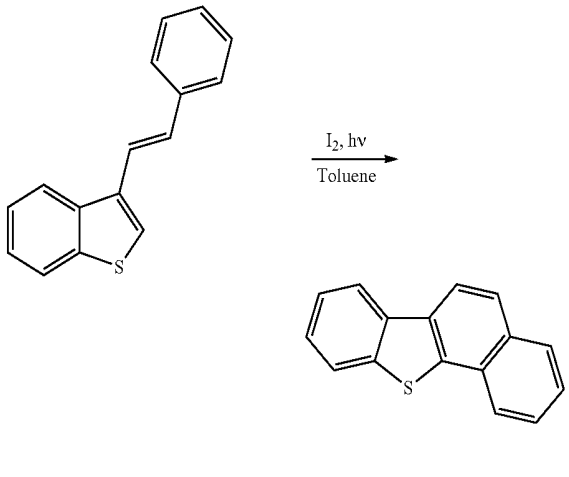
Example 1

Synthesis of 5-(3-(triphenylen-2-yl)phenyl)benzo[b] naphtho[2,1-d]thiophene (or Compound 69S)



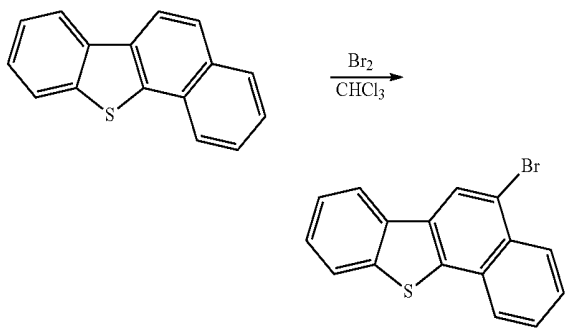
Synthesis of 3-styrylbenzo[b]thiophene

This is based on Journal of Heterocyclic Chemistry, 18(5), 967-72, 1981. NaH (1.3 g, 28 mmol) was added to a mixture of 3-carbaldehydebenzo[b]thiophene (4.27 g, 25 mmol), diethyl benzylphosphonate (5.76 g, 25 mmol) in 50 mL of 1,2-dimethoxyethane at 0° C. under N_2 and stirred for 15 minutes at 0° C. and 3 h at room temperature. The reaction mixture was then poured into ice water and filtrated. The solid from the filtration was recrystallized from ethanol to yield 4.5 g of desired product was obtained as a yellow solid.



Synthesis of benzo[b]naphtha[2,1-d]thiophene

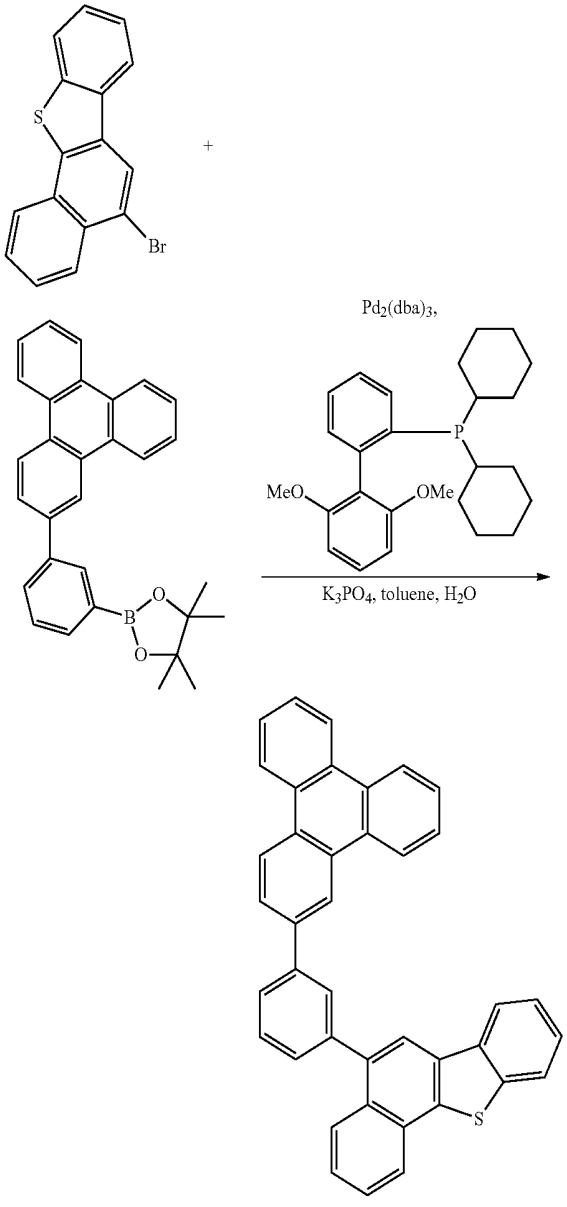
3-styrylbenzo[b]thiophene (13.8 g, 58 mmol), I_2 (0.13 g, 3 mmol) and 1.1 L of toluene were added in a photo reaction flask. The mixture was irradiated with a medium pressure mercury lamp with stirring for 6 h. The mixture was then concentrated and purified by silica gel column chromatography (15% EtOAc in hexanes). The product was further recrystallized from 20% EtOAc in methanol to give 12.9 g of pure product.



Synthesis of 5-bromobenzo[b]naphtho[2,1-d]thiophene

Br_2 (1.53 g, 9.4 mmol) in ~50 mL $CHCl_3$ was added dropwise to a solution of benzo[b]naphtha[2,1-d]thiophene (2.2 g,

9.4 mmol) in 300 mL of $CHCl_3$ at room temperature. The mixture was stirring for 22 h. The reaction was quenched by aqueous Na_2SO_3. After workup, silica gel column chromatography (50% CH_2Cl_2 in hexanes) and washing with minimum amount of methanol and hexane, 2.8 g of product was obtained.



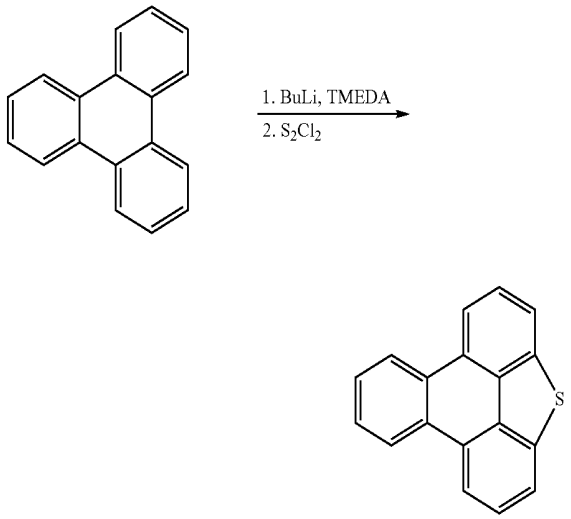
Compound 69S

Synthesis of Compound 69S

A mixture of 5-Bromobenzo[b]naphtho[2,1-d]thiophene (1.45 g, 4.6 mmol), 4,4,5,5-tetramethyl-2-(3-(triphenylen-2-yl)phenyl)-1,3,2-dioxaborolane (2.4 g, 5.58 mmol), K_3PO_4 (5.85 g, 27.6 mmol), 100 mL of toluene and 10 mL of water was bubbled with N_2 for 15 minutes. Then $Pd_2(dba)_3$ (212 mg, 0.23 mmol) and 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (378 mg, 0.92 mmol) were added. The mixture was bubbled with N_2 for another 20 minutes then brought to reflux for overnight. After workup, silica gel column chromatography (40% CH_2Cl_2 in hexanes), 2.2 g of product was obtained as a white solid. Compound 4S showed a triplet energy of 491 nm at 77K in 2-methylTHF.

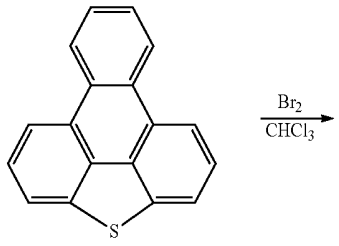
Example 2

Synthesis of 7-(3-(triphenylen-2-yl)phenyl)triphenyleno[1,12-bcd]thiophene (or Compound 67S)



Synthesis of triphenyleno[1,12-bcd]thiophene

To an oven-dried 3-necked 250 mL round bottom flask equipped with a condenser and two rubber septa was added 100 mL of dry hexanes via cannula. The flask was cooled to −50° C. using acetone/dry ice bath. TMEDA (3.3 mL, 21.0 mmol) was added via syringe followed by n-BuLi (1.6 M, 13.7 mL, 21.9 mmol) via syringe. The solution was allowed to warm to room temperature. After stirring for 30 minutes, triphenylene (1.0 g, 4.38 mmol) was added and heated to reflux under N_2. The mixture became dark red and was refluxed for 3 h. S_2Cl_2 (0.9 mL, 10.95 mmol) was added to the cooled solution. A violent reaction occurred followed by precipitation of a solid. Water was then added and the mixture was extracted twice with CH_2Cl_2. The organic extracts were dried over $MgSO_4$, filtered, and evaporated and the residue was purified by silica gel column chromatography (0-2.5% CH_2Cl_2 in hexanes). 0.5 g of triphenyleno[1,12-bcd]thiophene was collected.



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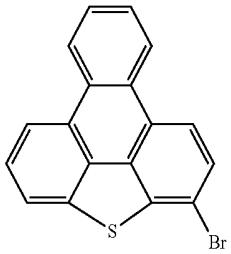
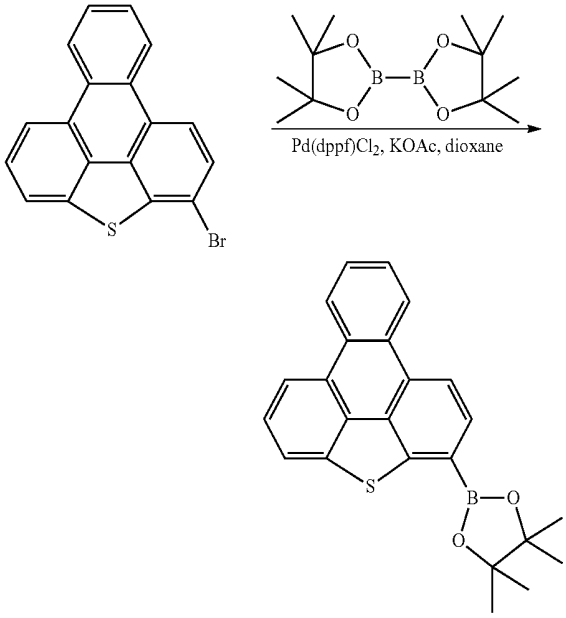


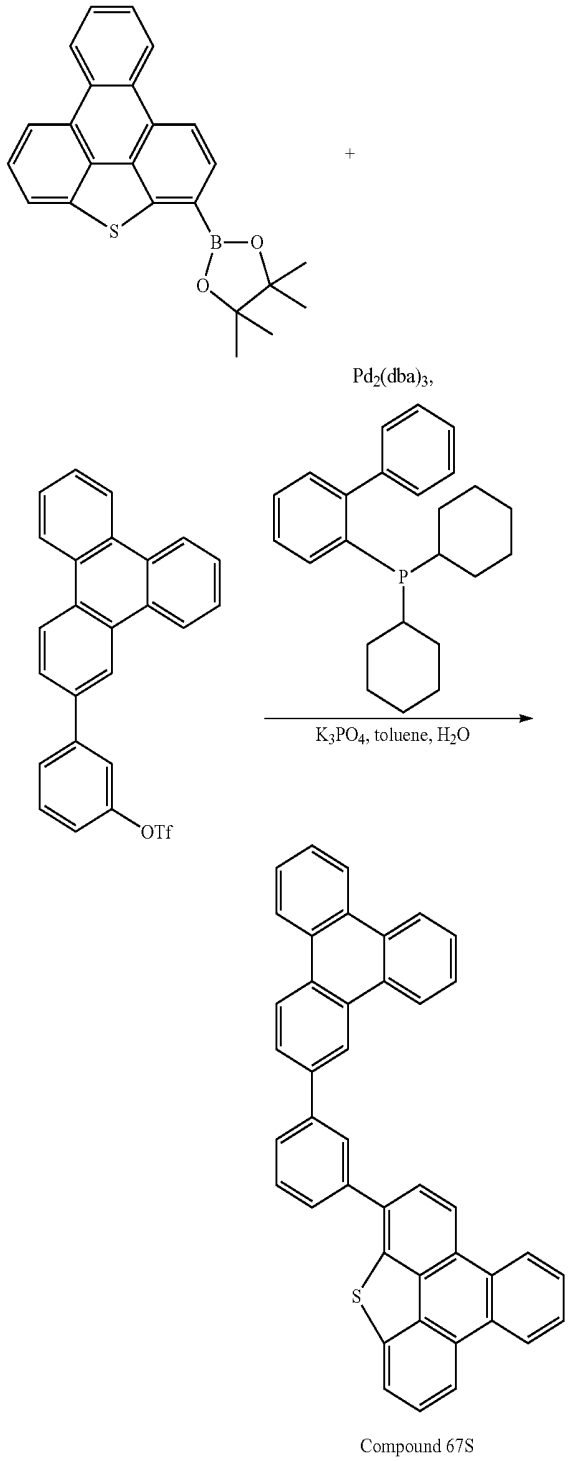
Synthesis of
7-bromotriphenyleno[1,12-bcd]thiophene

Triphenyleno[1,12-bcd]thiophene (1.5 g, 5.8 mmol) was dissolved in 100 mL of chloroform. Br_2 was slowly added into the reaction solution. After the reaction was stirred at room temperature for 3 days, the mixture was filtered through a Celite plug and washed by CH_2Cl_2. The combined filtrate was concentrated to get 2.2 g of 7-bromotriphenyleno[1,12-bcd] thiophene which was used for next step without further purification.



Synthesis of 4,4,5,5-tetramethyl-2-(triphenyleno[1, 12-bcd]thiophen-3-yl)-1,3,2-dioxaborolane

A mixture of 7-bromotriphenyleno[1,12-bcd]thiophene (2.2 g, 6.5 mmol), KOAc (1.6 g, 20 mmol) and 300 mL of dioxane was bubbled with N_2 for 25 minutes. Then Pd(dppf) Cl_2 (0.16 g, 0.2 mmol) was added and the mixture was bubbled with N_2 for another 25 minutes. The reaction was heated to 90° C. overnight. The mixture was then cooled to temperature, filtered through a Celite plug and washed by CH_2Cl_2. The combined filtrate was concentrated. The crude product was purified by silica gel silica column chromatography (3% EtOAc in hexanes) as elute to yield 0.25 g of product.



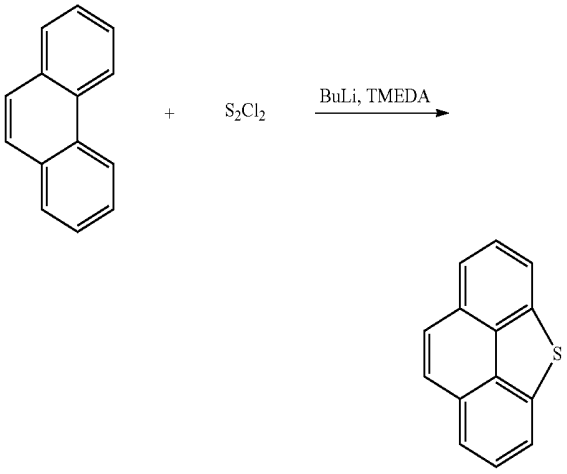
Synthesis of Compound 67S

A mixture of 4,4,5,5-tetramethyl-2-(triphenyleno[1,12-bcd]thiophen-7-yl)-1,3,2-dioxaborolane (0.24 g, 0.62 mmol), 3-(triphenylen-2-yl)phenyl trifluoromethanesulfonate (0.26 g, 0.57 mmol), K_3PO_4 (0.36 g, 1.7 mmol), dioxane (30 mL) and water (3 mL) was bubbled with N_2 for 1 h. Then $Pd_2(dba)_3$ (5.2 mg, 0.0057 mmol) and (biphenyl-2-yl)dicyclohexylphosphine (8 mg, 0.023 mmol) was added and the mixture was bubbled with N_2 for another 15 minutes. After stirring at room temperature overnight, additional Pd_2 $(dba)_3$ (5.2 mg, 0.0057 mmol) and (biphenyl-2-yl)dicyclo-

hexylphosphine (8 mg, 0.023 mmol) were added. The reaction was stirred at room temperature for three days. The precipitate was collected by filtration and purified by silica gel column chromatography (0-40% of CH_2Cl_2 in hexanes) to yield 50 mg of product as a white solid that showed a triplet energy of 490 nm at 77 K in 2-methylTHF.

Example 3

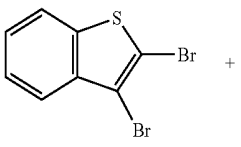
Synthesis of Phenanthro[4,5-bcd]thiophene



The synthesis is based on Heteroatom Chemistry, 5(2), 113-19, 1994. To an oven-dried 3-neck 1 L round bottom flask equipped with a condenser and a dropping funnel was added phenanthrene (5.7 g, 32 mmol) and 220 mL of dry hexanes. TMEDA (24 mL, 160 mmol) was added followed by n-BuLi (1.6 M, 100 mL, 160 mmol) dropwise via a dropping funnel. The solution was heated to reflux for 3 h under N_2. The reaction mixture was cooled in an ice bath and S_2Cl_2 (6.4 mL, 80.0 mmol) was added slowly. The reaction mixture was allowed to stir overnight at room temperature. Water and CH_2Cl_2 were added and the layers were separated. The aqueous layer was extracted with CH_2Cl_2. The organic extracts were dried over $MgSO_4$, filtered, and evaporated. The material was purified by silica gel column chromatography (0-10% CH_2Cl_2 in hexanes) to yield 2.3 g of an off-white solid contaminated with sulfur. Another column chromatography eluting with hexanes provided 0.42 g of pure material. Phenanthro[4,5-bcd]thiophene showed a triplet energy of 508 nm at 77K in 2-methylTHF.

Example 4

Synthesis of Benzo[b]phenanthro[9,10-d]thiophene



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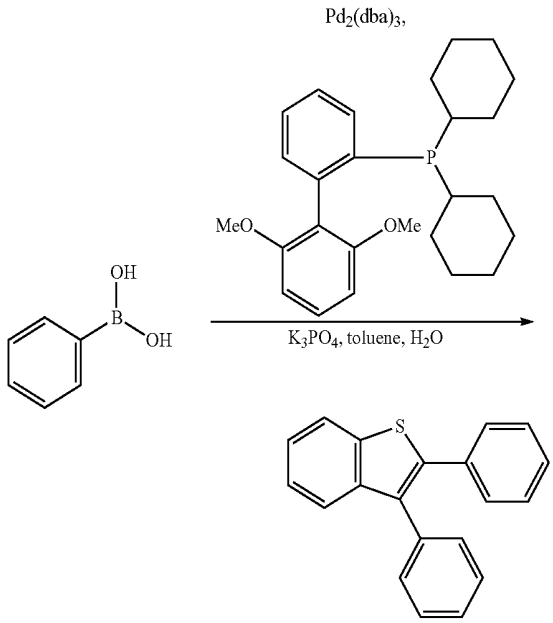
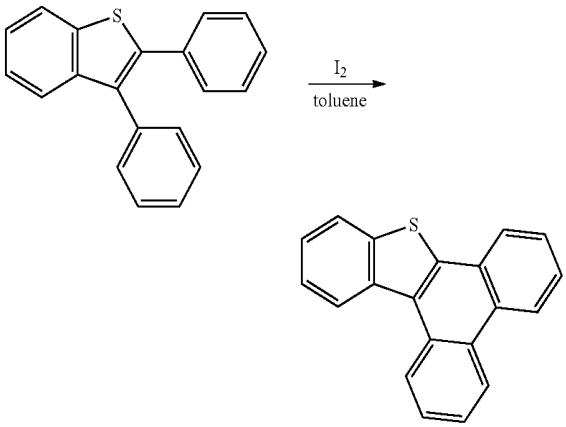


The synthesis is based on Tetrahedron, 37(1), 75-81, 1981. To a 500 mL 3-neck round bottom flask was added 2,3-dibromobenzo[b]thiophene (5.0 g, 17.12 mmol), phenylboronic acid (5.2 g, 42.81 mmol), 2-dicyclohexylphosphino-2', 6'-dimethoxybiphenyl (281 mg, 0.68 mmol), K_3PO_4 (11.8 g, 51.36 mmol), 150 mL of toluene and 5 mL of water. N_2 was bubbled directly into the flask for 20 minutes. $Pd_2(dba)_3$ (157 mg, 0.171 mmol) was added to the reaction mixture which was then heated to reflux for 5 h. Water was added to the cooled reaction mixture and the layers were separated. The aqueous layer was extracted twice with CH_2Cl_2 and the organic extracts were dried over $MgSO_4$, filtered, and evaporated to yield a red oil which was dried to give 5.71 g of a red solid. The solid was purified by silica gel column chromatography (10-20% CH_2Cl_2 in hexanes) to yield 4.81 g of the product as a white solid.

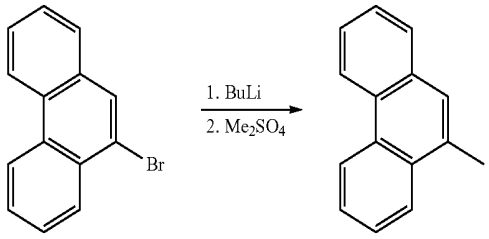


A photoreactor was loaded with 2,3-diphenylbenzo[b] thiophene (4.81 g, 16.8 mmol) and 800 mL toluene. The solution was irradiated using a medium pressure mercury lamp for 12 h. The solvent was evaporated and the residue was purified by silica gel column chromatography (0-20% of EtOAc in hexanes). The product was collected and recrystallized from hexanes (with a small amount of EtOAc to initially dissolve the material) to yield 1.61 g of product an off-white

solid. Benzo[b]phenanthro[9,10-d]thiophene showed a triplet energy of 488 nm at 77 Kin 2-methylTHF.

Example 5

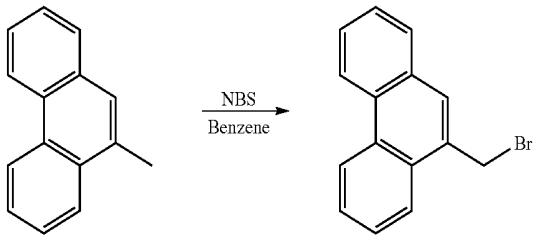
Synthesis of benzo[b]triphenyleno[2,1-d]thiophene



This synthesis is based on Journal of Heterocyclic Chemistry, 21(6), 1775-9, 1984.

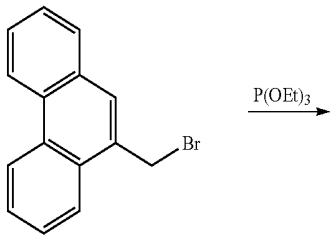
Synthesis of 9-methylphenanthrene

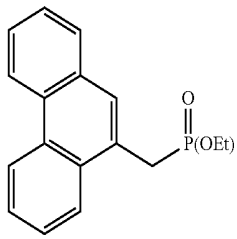
9-Bromophenanthrene (27 g, 102 mmol) was dissolved in 400 mL of dry ether and cooled to −78° C. 170 mL of BuLi (1.6 M in hexane) was slowly added into this solution in 45 minutes. The reaction mixture was warmed to room temperature. The mixture was then stirred at room temperature for 2 h before it was cooled to −78° C. again and Me_2SO_4 (17.6 g, 133 mmol) in ether was slowly added. The mixture was stirred at room temperature for 10 h. The mixture was poured into 15% HCl aqueous solution and extracted with CH_2Cl_2 and dried over $MgSO_4$. The solvent was evaporated to give a residue which was recrystallized from hexane to yield 14.2 g of product as a white solid.



Synthesis of 9-(bromomethyl)phenanthrene

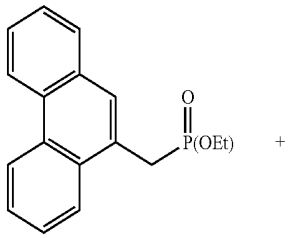
A mixture of 9-methylphenanthrene (14.2 g, 74 mmol), benzoyl peroxide (40 mg, 0.16 mmol) and NBS (13.3 g, 74.6 mmol) in 210 mL of benzene was refluxed for 5 h. The reaction mixture was cooled to 0° C. and the succinimide precipitated was removed by filtration. The filtrate was washed by 15% NaOH, dried over $MgSO_4$ and concentrated to yield 18 g of product which was used for the next step without further purification.





Synthesis of diethyl (phenanthren-9-ylmethyl)phosphonate

9-(Bromomethyl)phenanthrene (18 g, 66.4 mmol) and triethyl phosphite (10.7 g) were mixed and heated to 150° C. under N_2 for 4 h. The reaction mixture was concentrated and the residue was purified by silica gel column chromatography to yield 12 g of product.



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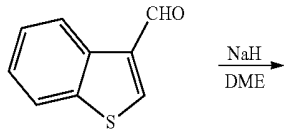
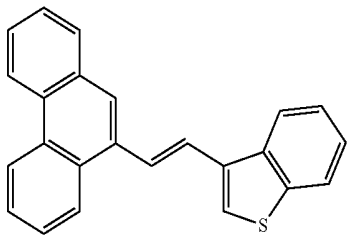
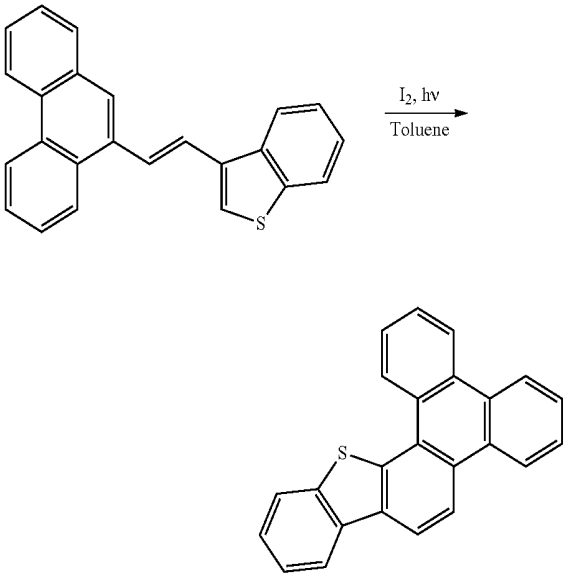




Synthesis of 3-(2-(phenanthren-9-yl)vinyl)benzo[b]thiophene

Diethyl(phenanthren-9-ylmethyl)phosphonate (11 g, 33.5 mmol) and 3-carbaldehydebenzo[b]thiophene (5.5 g, 33.5

mmol) were dissolved in 250 mL of 1,2-dimethoxyethane. The mixture was cooled to 0° C. and NaH (6 g, 150 mmol) was added in portions. The reaction mixture was warmed to room temperature and heated to reflux for 2.5 h. The reaction mixture was concentrated and the residue was purified by silica gel column chromatography (30% CH_2Cl_2 in hexane) to yield 6 g of product.



Synthesis of benzo[b]triphenyleno[2,1-d]thiophene

3-(2-phenanthren-9-yl)vinyl)benzo[b]thiophene (0.5 g, 1.5 mmol), I_2 (38 mg, 0.15 mmol) and 250 mL of toluene were charged in a photo reactor. The reaction mixture was irradiated with a medium pressure mercury lamp for 3.5 h. The reaction mixture was concentrated to give a residue which was purified by silica gel chromatography (10% CH_2Cl_2 in hexanes) to yield 0.3 g of product. Benzo[b]triphenyleno[2,1-d]thiophene showed a triplet energy of 463 nm at 77K in 2-methylTHF.

Device Examples

All example devices were fabricated by high vacuum (<10^{-7} Torr) thermal evaporation. The anode electrode was 1200 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1,000 Å of Al. All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H_2O and O_2) immediately after fabrication, and a moisture getter was incorporated inside the package.

The organic stack of Device Examples 1-4 in Table 1 consisted of sequentially, from the ITO surface, 100 Å of Compound A as the hole injection layer (HIL), 300 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (α-NPD) as the hole transporting layer (HTL), 300 Å of Compound 4S doped with 10 or 15 wt % of Compound A as the emissive layer (EML), 100 Å or 50 Å of Compound 69S or Compound B as the ETL2 and 400 Å or 450 Å of Alq_3 (tris-8-hydroxyquinoline aluminum) as the ETL1.

Comparative Device Example 1 was fabricated similarly to the Device Example 3 except that the CBP was used as the host.

The device data for the Device Examples and Comparative Device Examples is shown in Table 2. Ex. is an abbreviation for example. Comp. is an abbreviation for comparative. Cmpd. is an abbreviation for compound.

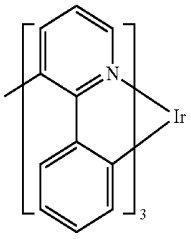
TABLE 2

Device Example and Comparative Device Example data.

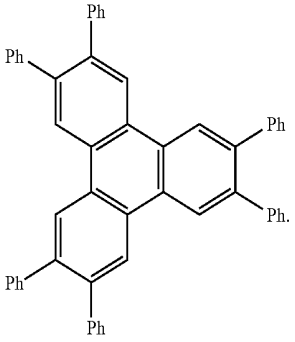
				at 1000 cd/m²						at 40 mA/cm²	
Device Ex.	Cmpd. A %	ETL2 (Å)	ETL1 (Å)	x	x	V (V)	LE (cd/A)	EQE (%)	PE (lm/W)	L_0 (cd/m²)	LT_{80} (h)
1	10	69S (100)	Alq_3 (400)	0.371	0.595	7.2	31	8.6	13.5	8,878	80
2	15	69S (100)	Alq_3 (400)	0.369	0.598	6.9	34.6	9.6	15.7	9,816	141
3	10	B (50)	Alq_3 (450)	0.369	0.598	6.5	35.5	9.8	17.1	9,497	72
4	15	B (50)	Alq_3 (450)	0.367	0.602	6.1	46.8	12.9	24.1	11,974	95
Comp. Ex. 1	10	B (50)	Alq_3 (450)	0.345	0.615	5.8	61	16.7	33.0	16,118	82

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

Compound A



Compound B



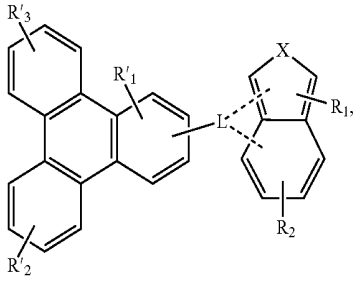
Device Examples use Compound 69S as the host. The external quantum efficiencies are 8.8-12.9%, which is lower than the efficiency of the Comparative Device Example which uses CBP as the host. The reason may be a certain degree of luminescence quenching of the phosphorescence of Compound A by Compound 69S due to the similar triplet energy (Compound 69S T_1=491 nm; Compound A T_1=525 nm). However, the operational lifetime of the Device Examples are respectable compared to that of the Comparative Device Example. Device Example 2 has a LT_{80} (time required for the initial luminance L_0 to drop from 80%) of 141 h whereas Comparative Device Example 1 has a LT_{80} of 82 h. The result demonstrates the stability of the triphenylene-benzo-/dibenzo-moiety compounds with fused rings. Since the triplet energy of triphenylene-benzo-/dibenzo-moiety compounds with benzo fused rings may be lower than 490 nm, they may be particularly suitable as host materials for yellow, orange, red or IR phosphorescent emitters.

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

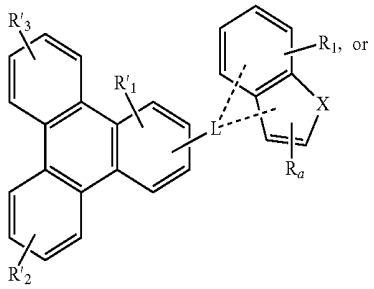
The invention claimed is:

1. A compound comprising one of the formulae:

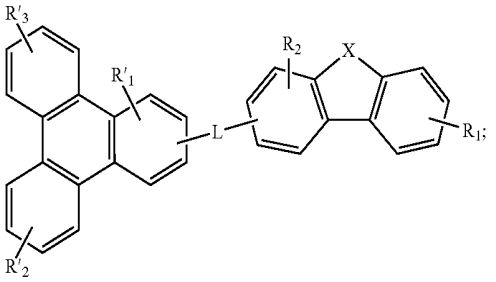
Formula 2



Formula 3



Formula 4



wherein X is S or Se;

wherein R_1, R_2, and R_a are independently selected from hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl;

wherein each of R_1 and R_2 represent mono, di, tri or tetra substituents;

wherein at least two substituents of R_1 or R_2 are joined to form a fused ring;

wherein R_a represents mono or di substituents which cannot fuse to form a benzo ring; and

wherein L represents a spacer or a direct connection to the benzothiophene, or benzoselenophene moiety with additional fused rings;

wherein R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl;

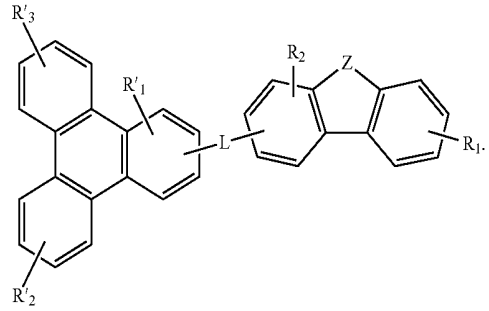
wherein each of R'_1, R'_2, and R'_3 may represent mono, di, tri, or tetra substituents.

2. The compound of claim **1**, wherein the at least two substituents of R_1 or R_2 are joined to form a 6-membered carbocyclic or heterocyclic ring.

3. The compound of claim **2**, the at least two substituents of R_1 or R_2 are joined to form a benzene ring.

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

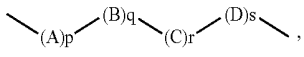
Formula 4



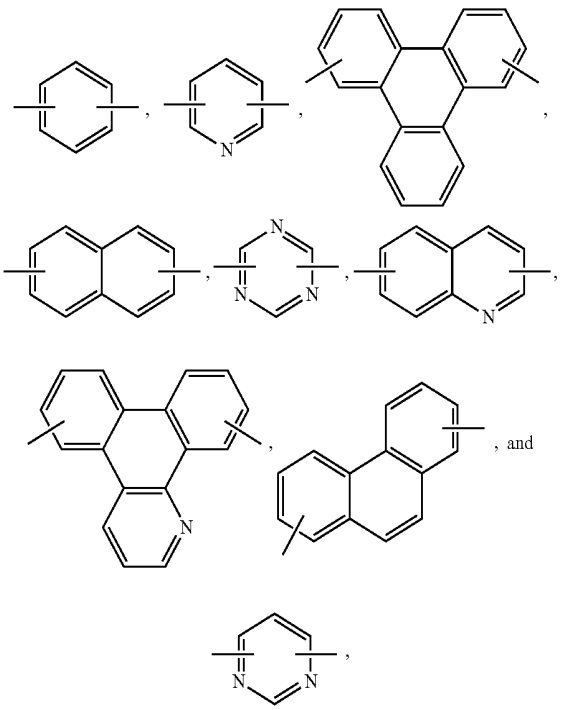
5. The compound of claim **1**, wherein X is S.

6. The compound of claim **1**, wherein L is a direct connection.

7. The compound of claim **1**, wherein L has the formula:



wherein A, B, C and D are independently selected from the group consisting of:



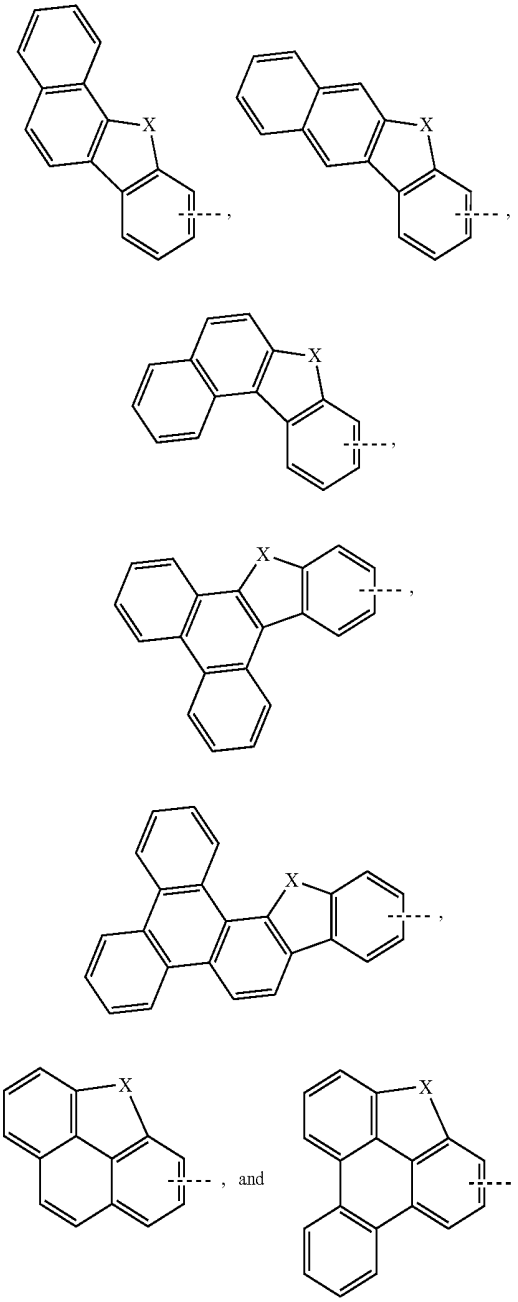
wherein A, B, C and D are optionally further substituted with R_a;

wherein each of p, q, r and s are 0, 1, 2, 3, or 4; and

wherein p+q+r+s is at least 1.

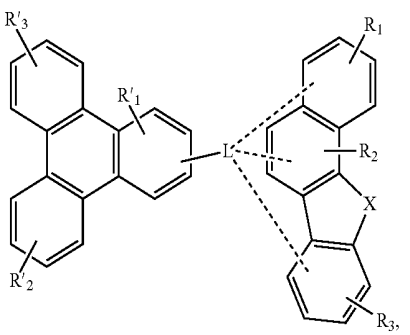
8. The compound of claim **1**, wherein L is phenyl.

9. The compound of claim **1**, wherein the at least two substituents of R_1 or R_2 that are joined to form fused rings form a ring system selected from the group consisting of:



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

Formula 4-1



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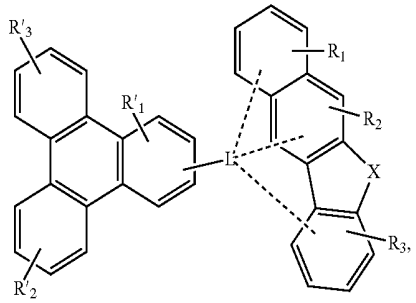
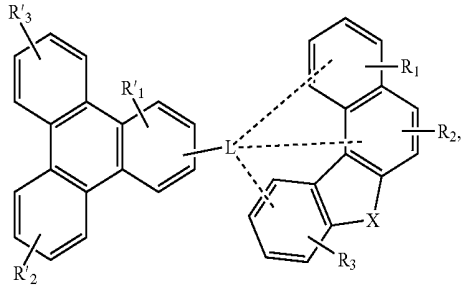
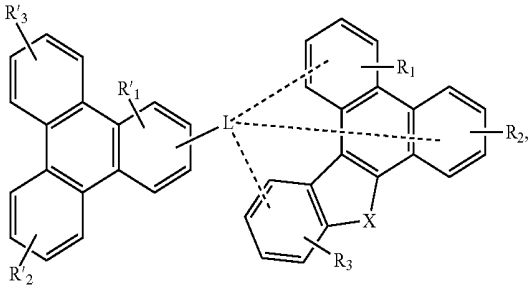
Formula 4-2



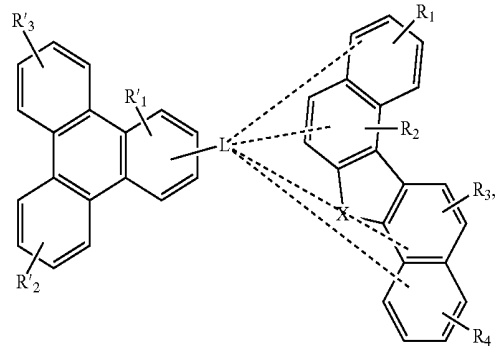
Formula 4-3



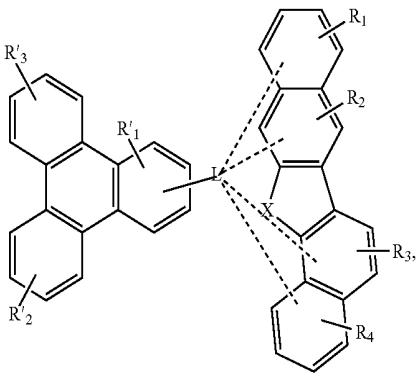
Formula 4-4



Formula 4-5



Fromula 4-6



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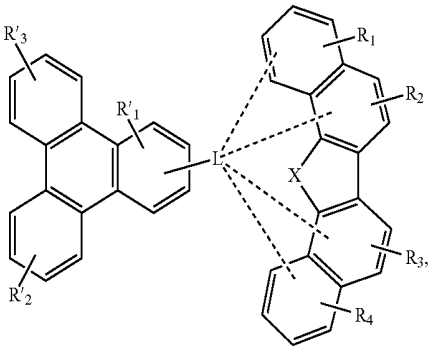
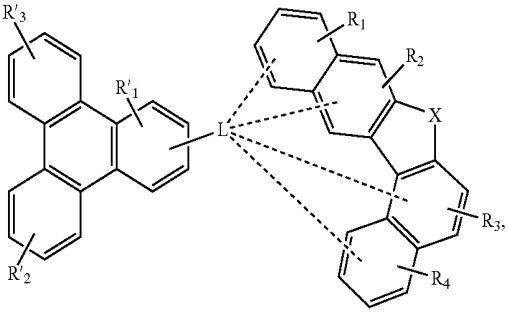
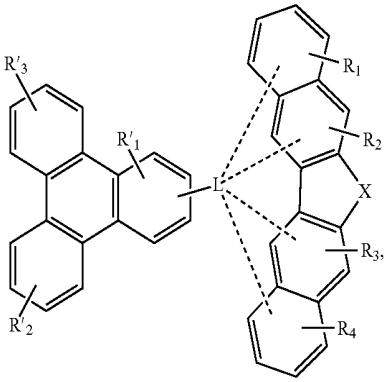
Formula 4-7



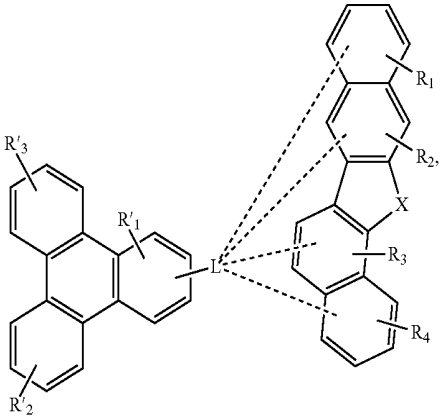
Formula 4-8



Formula 4-9



Formula 4-10



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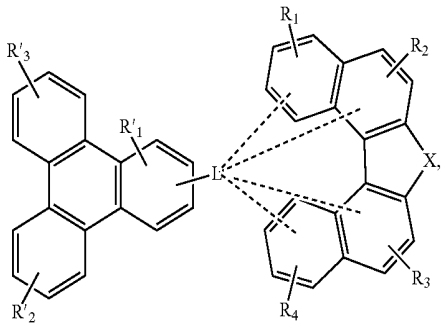
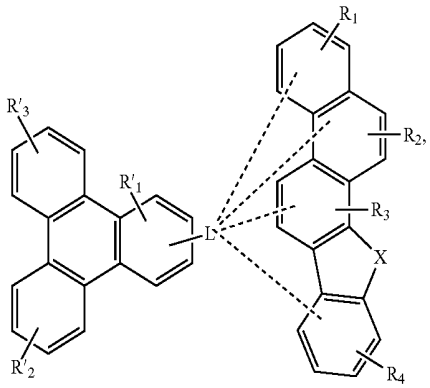
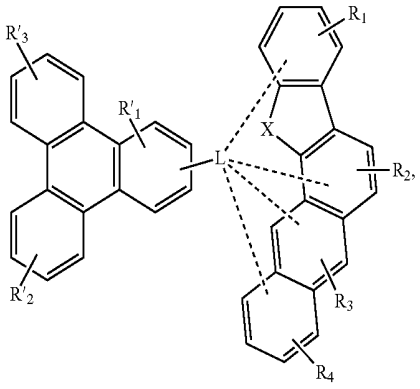
Formula 4-11



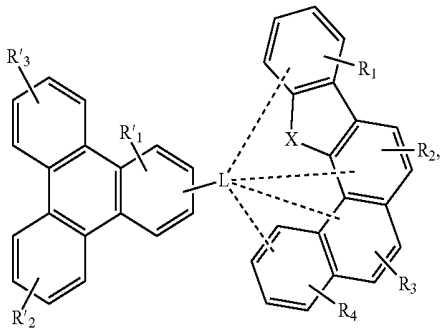
Formula 4-12



Formula 4-13



Formula 4-14



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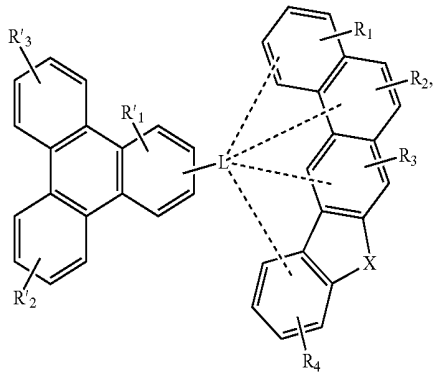

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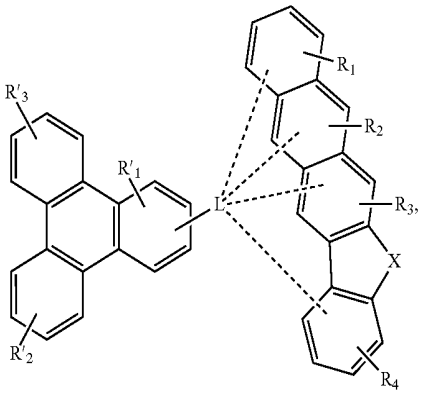
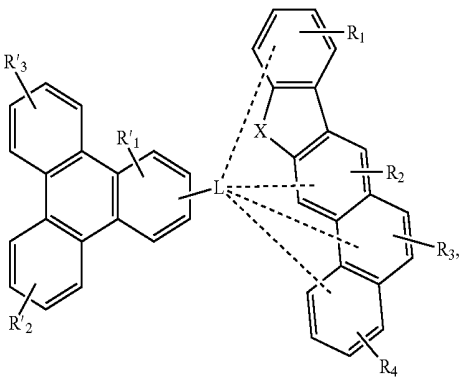
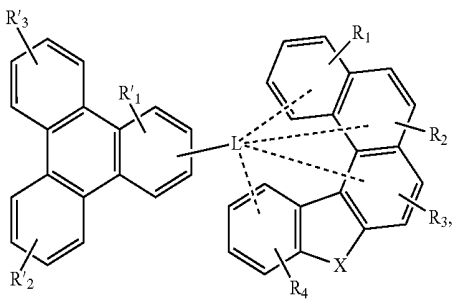


Formula 4-17



Formula 4-18



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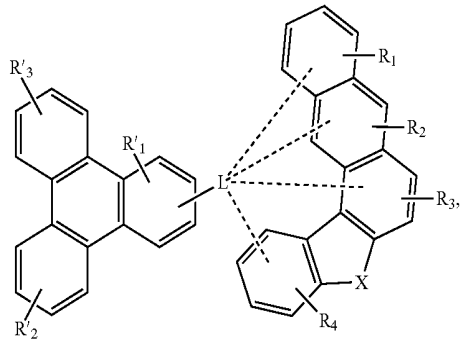
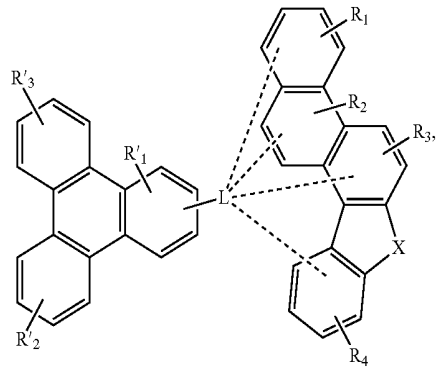
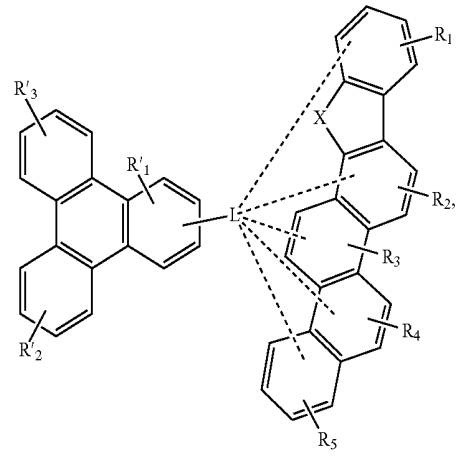
Formula 4-19



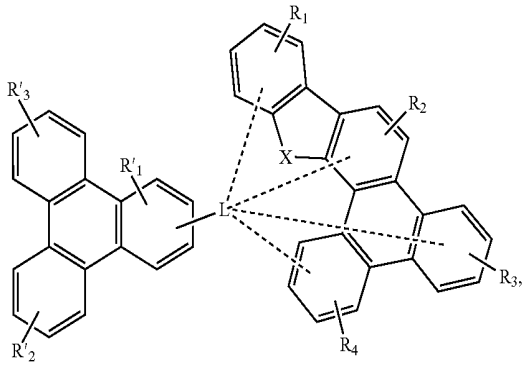
Formula 4-20



Formula 4-21



Formula 4-22



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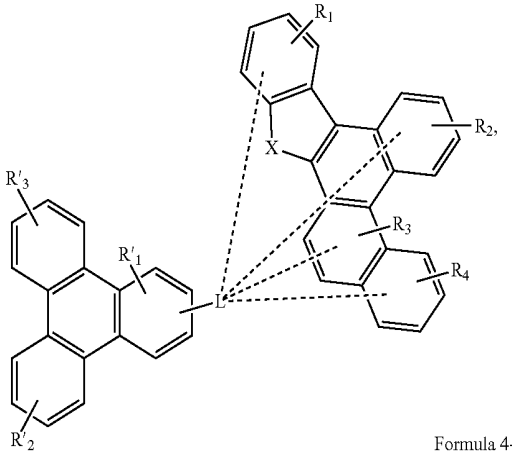
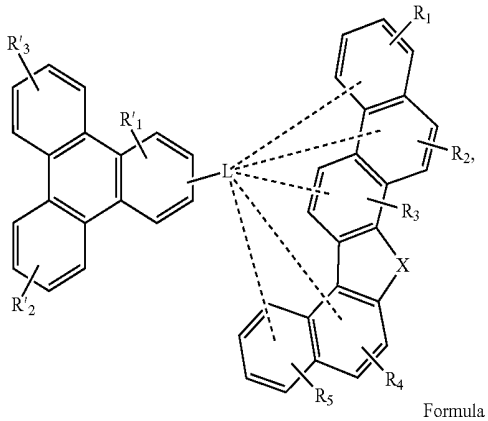
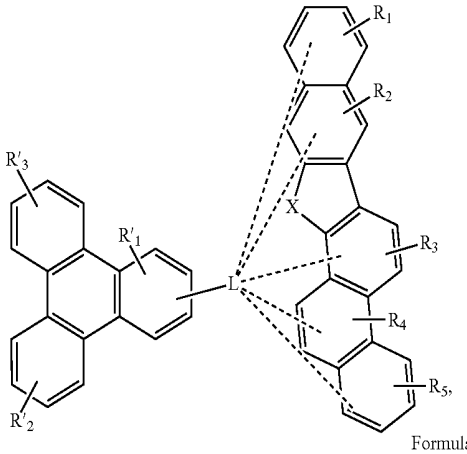
Formula 4-23



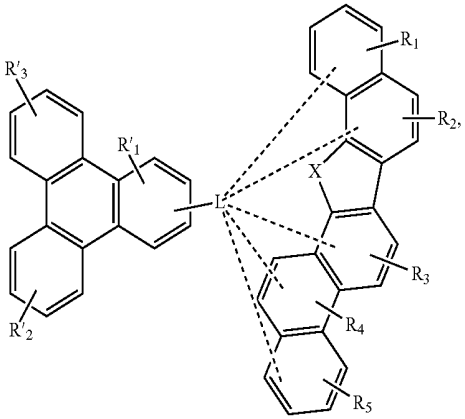
Formula 4-24



Formula 4-25



Formula 4-26



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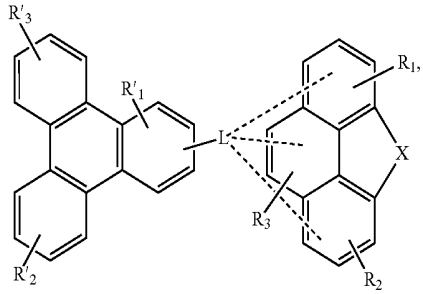
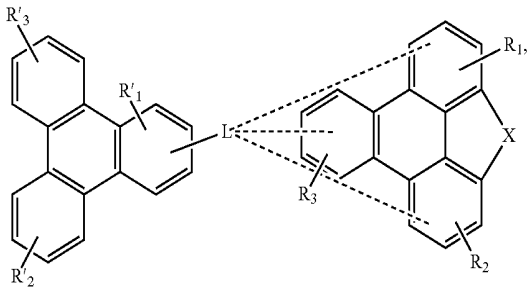
Formula 4-27



Formula 4-28



wherein X is S or Se;

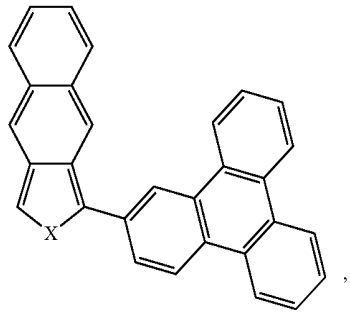
wherein R_1, R_2, R_3, R_4, R_5, R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl;

wherein each of R_1, R_2, R_3, R_4, R_5, R'_1, R'_2, and R'_3 may represent mono, di, tri or tetra substituents; and

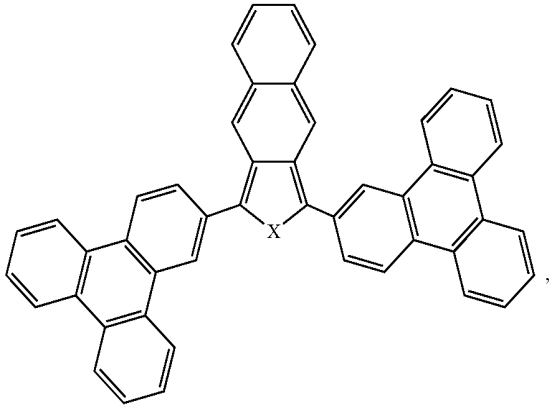
wherein L is a spacer or a direct linkage.

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

Compound 3



Compound 4



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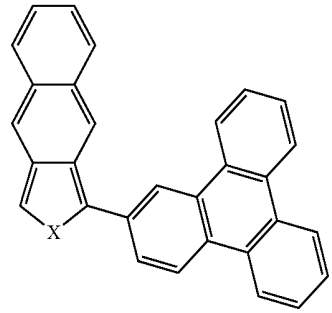
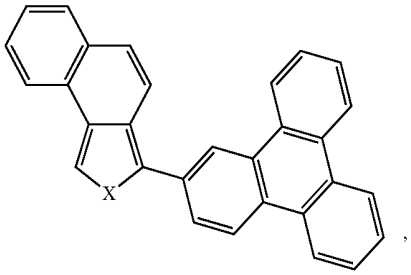
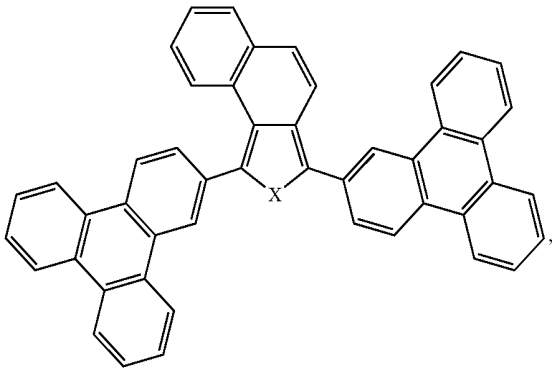
Compound 3



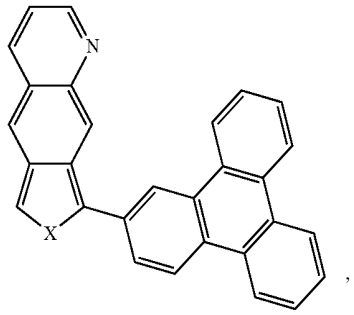
Compound 5



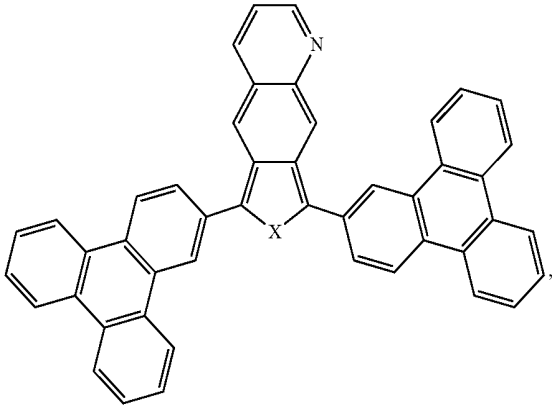
Compound 6



Compound 7



Compound 8



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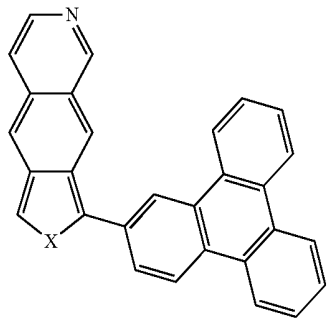
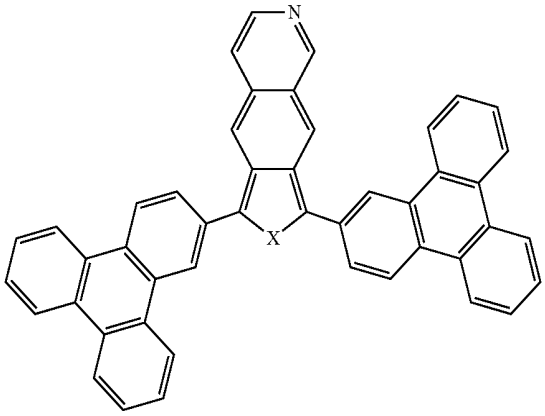
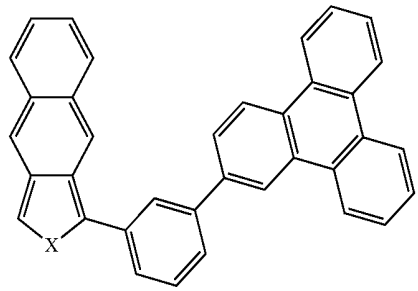
Compound 9



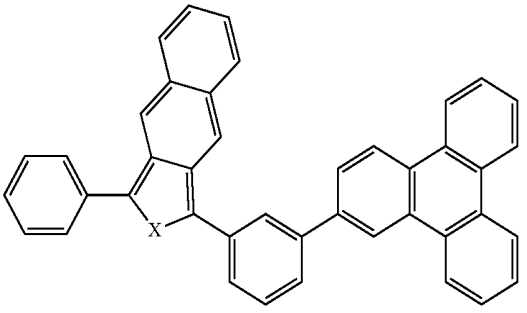
Compound 10



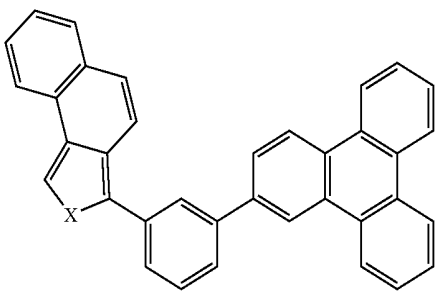
Compound 11



Compound 12



Compound 13



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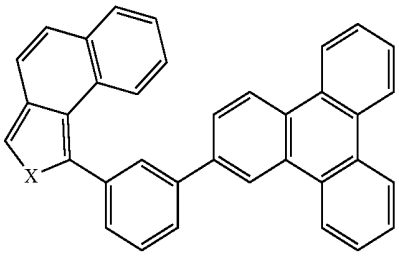
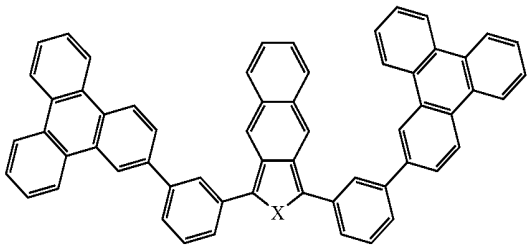
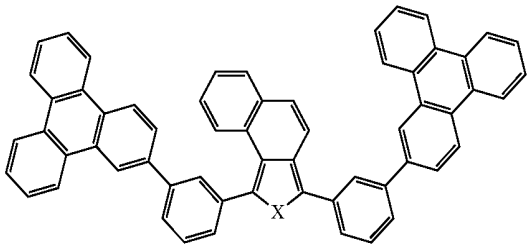
Compound 14



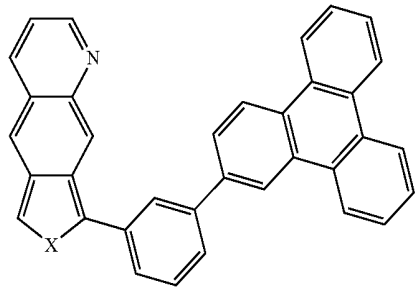
Compound15



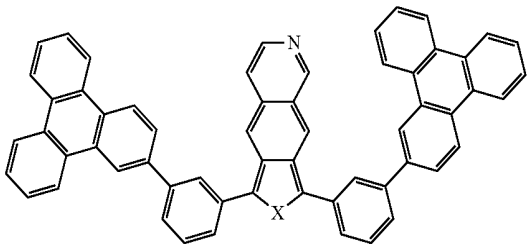
Compound 16



Compound 17



Compound 18



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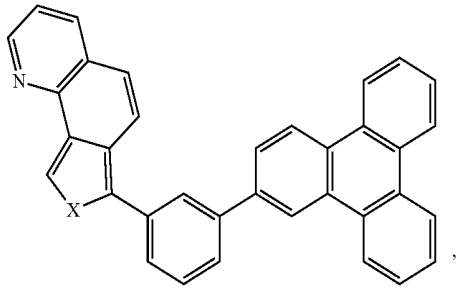
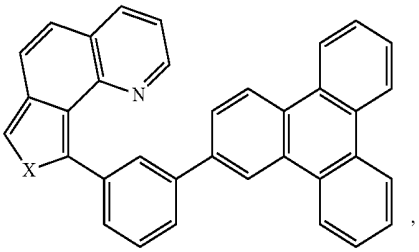
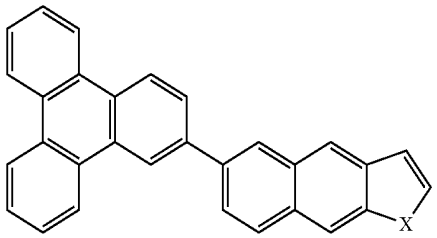
Compound 19



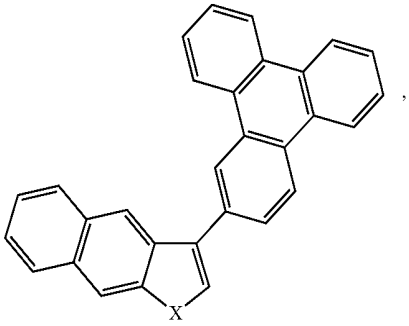
Compound 20



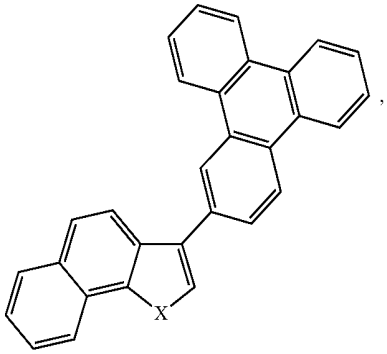
Compound 21



Compound 22



Compound 23



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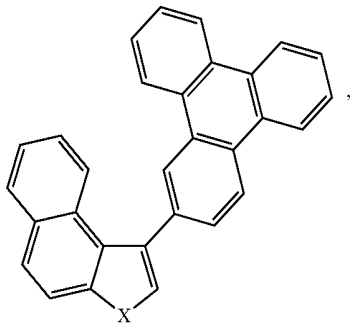
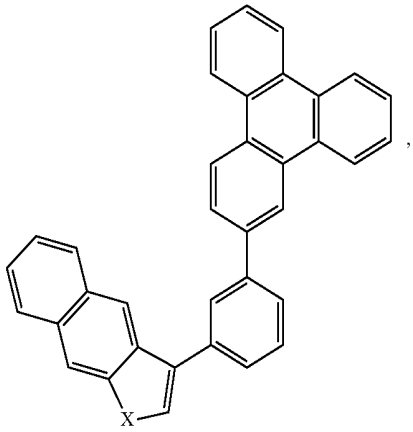
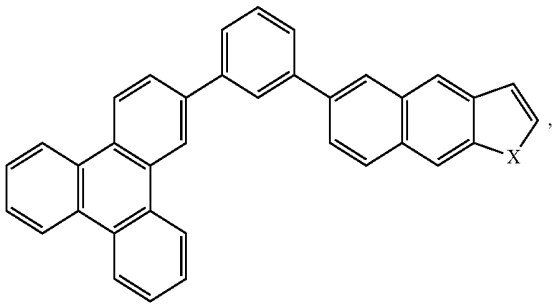
Compound 24



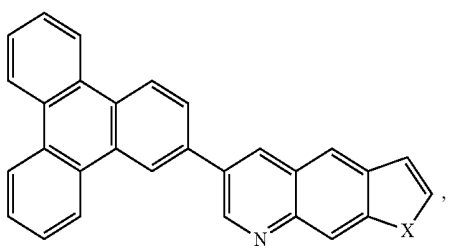
Compound 25



Compound 26



Compound 27



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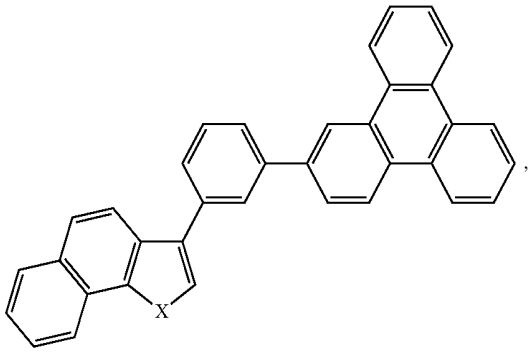
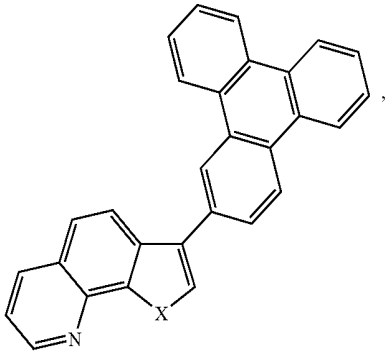
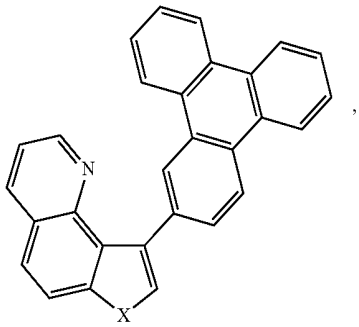
Compound 28



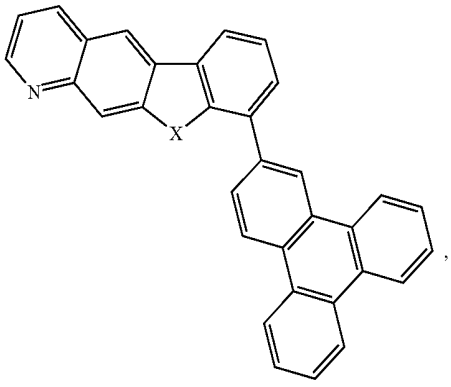
Compound 29



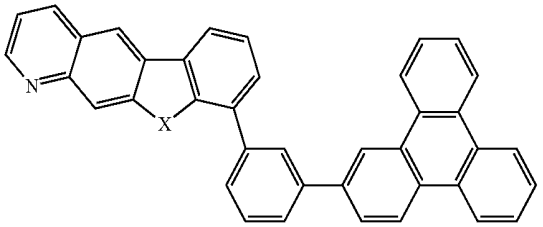
Compound 30



Compound 31



Compound 32



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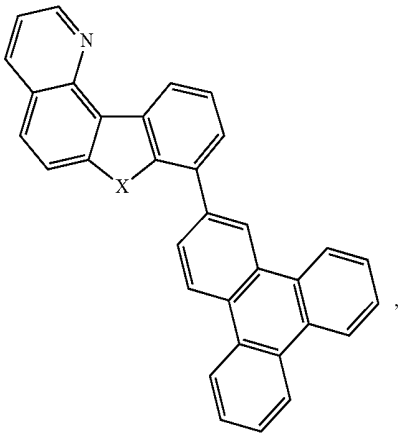
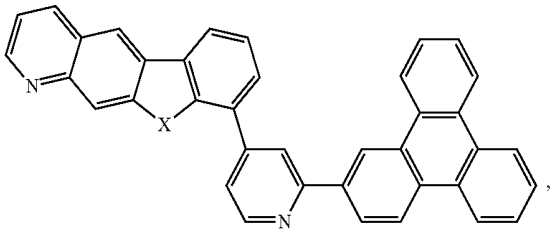
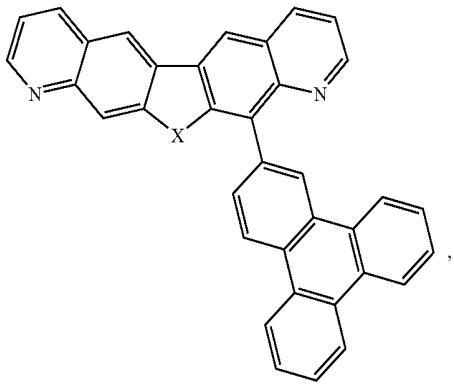
Compound 33



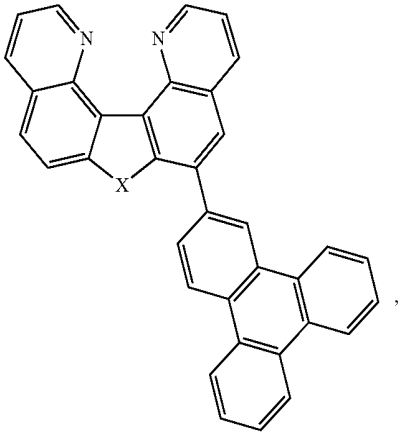
Compound 34



Compound 35



Compound 36



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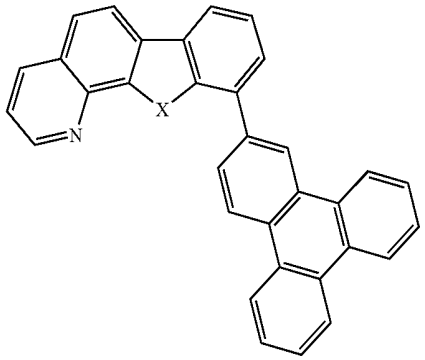
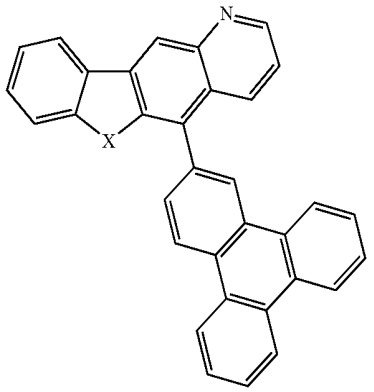
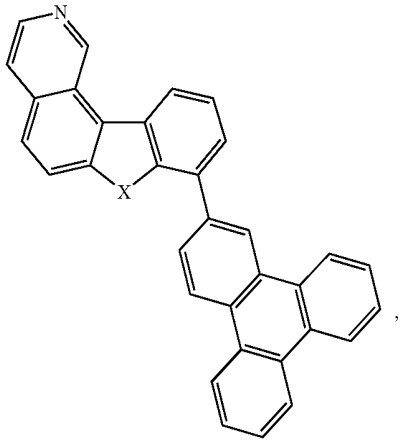
Compound 37



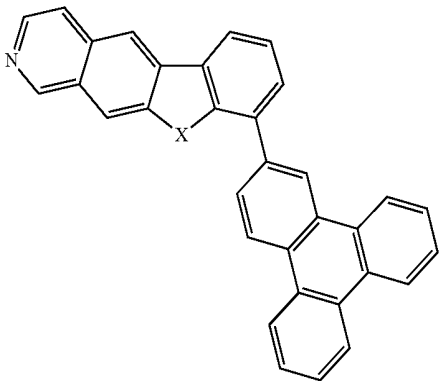
Compound 38



Compound 39



Compound 40



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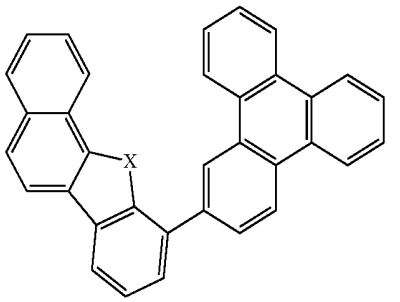
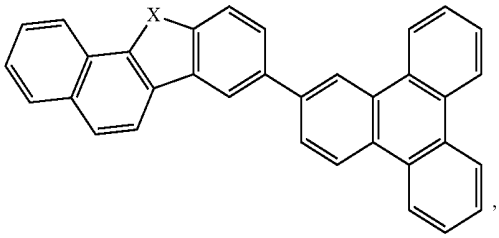
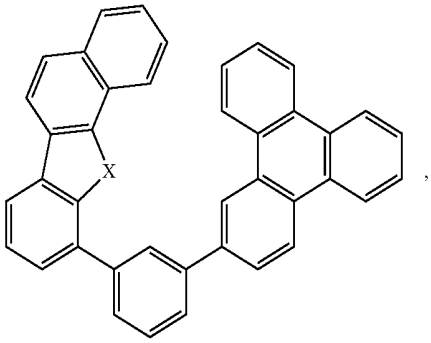
Compound 41



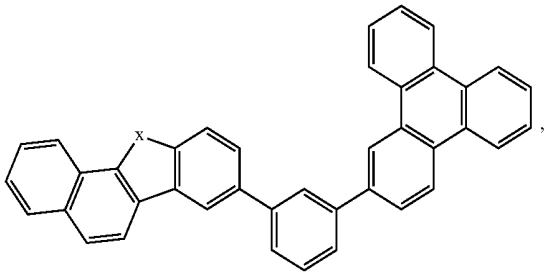
Compound 42



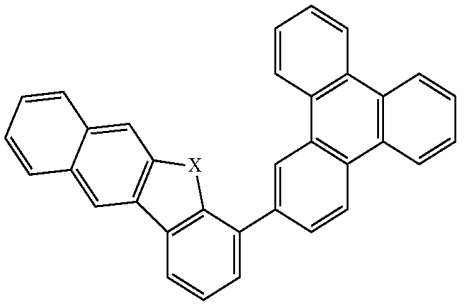
Compound 43



Compound 44



Compound 45



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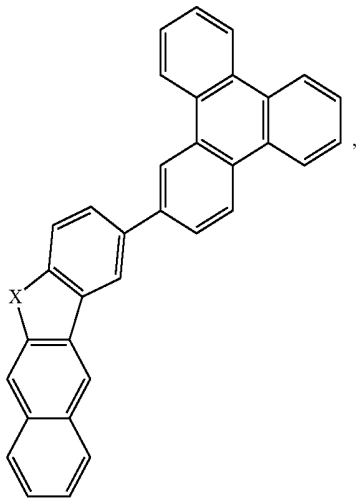
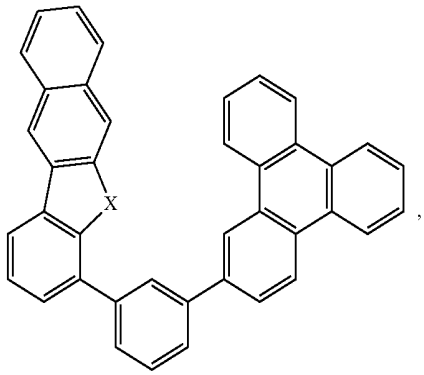
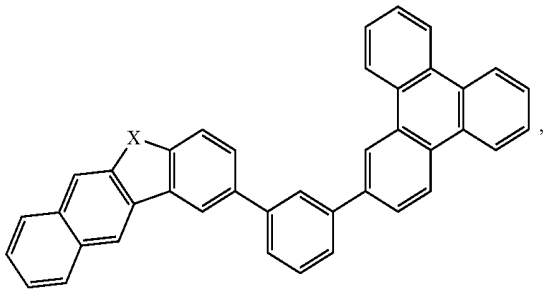
Compound 46



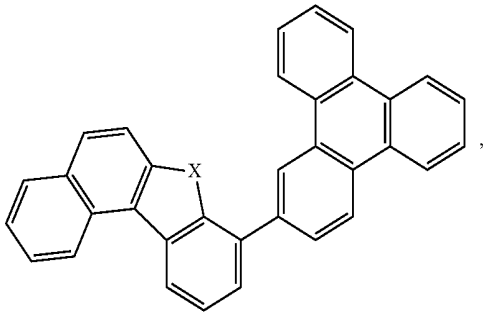
Compound 47



Compound 48



Compound 49



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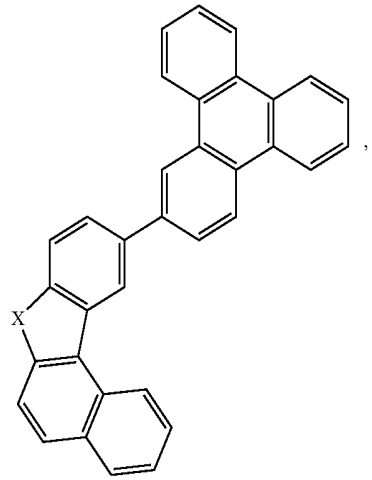
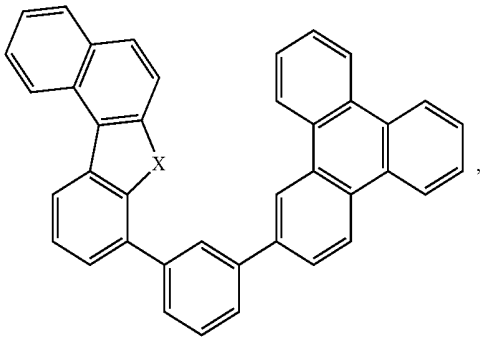
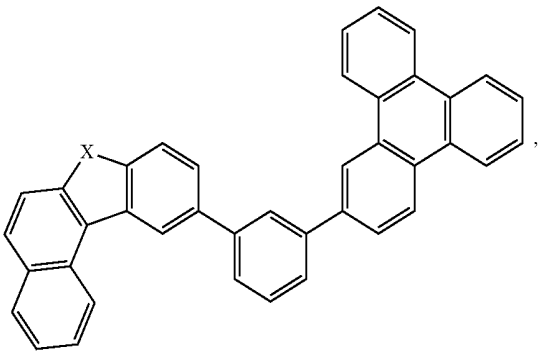
Compound 50



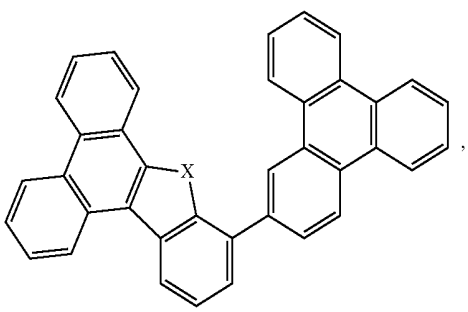
Compound 51



Compound 52



Compound 53



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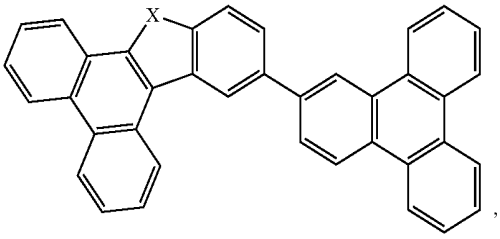
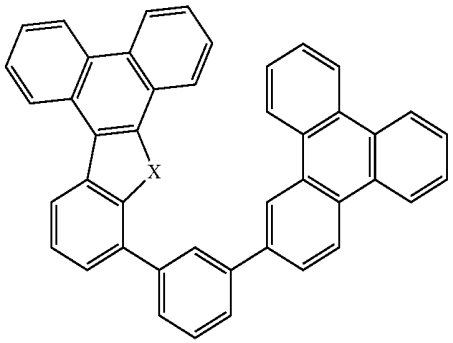
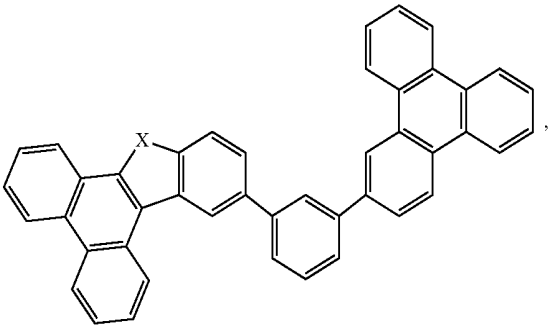
Compound 54



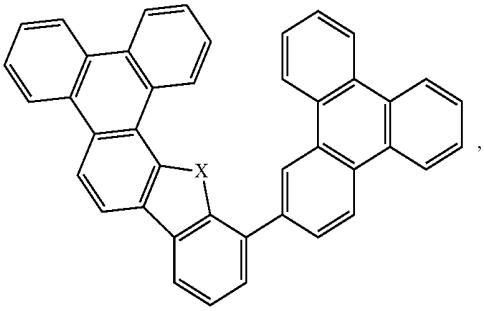
Compound 55



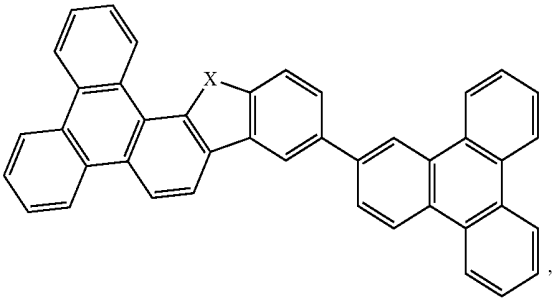
Compound 56



Compound 57



Compound 58



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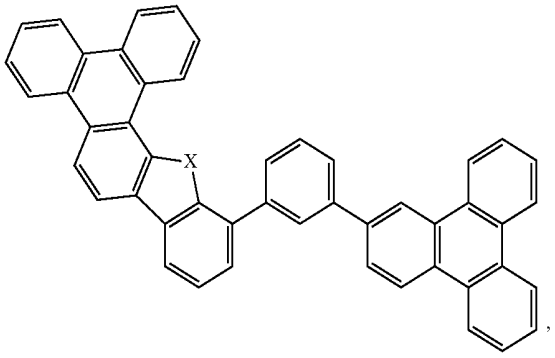
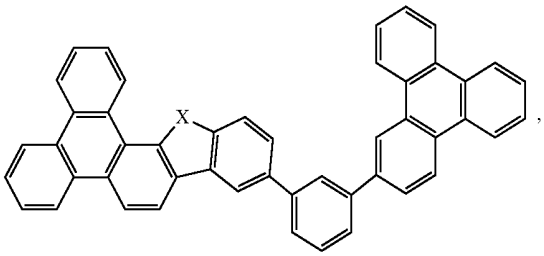
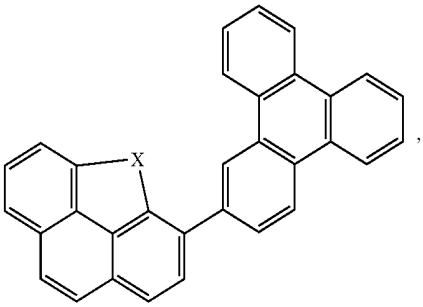
Compound 59



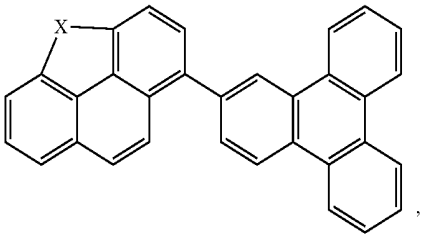
Coumpound 60



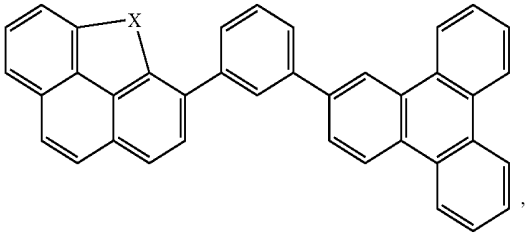
Compound 61



Compound 62

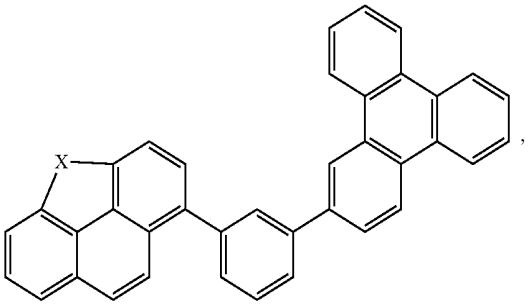


Compound 63

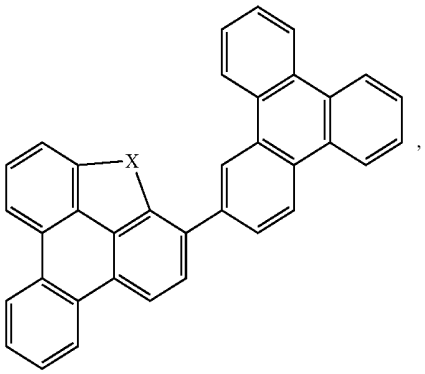


-continued

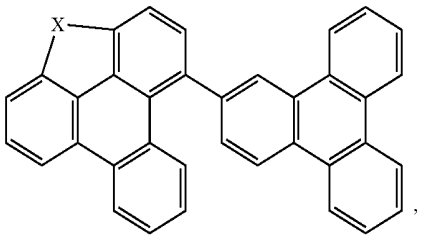
Compound 64



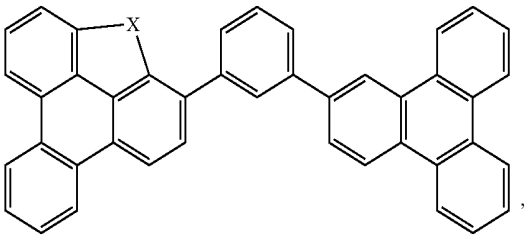
Compound 65



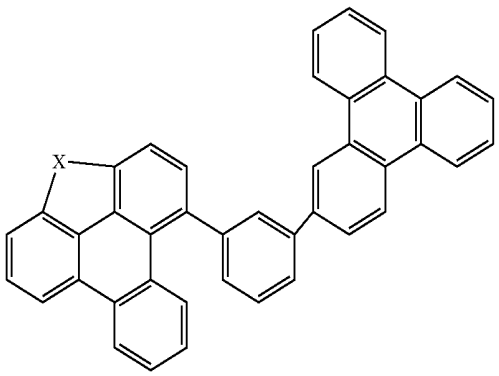
Compound 66



Compound 67



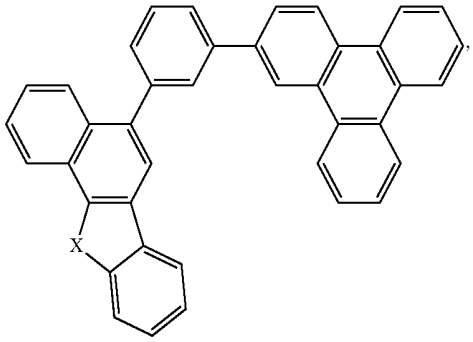
Compound 68



, and

-continued

Compound 69



wherein X is S, or Se.

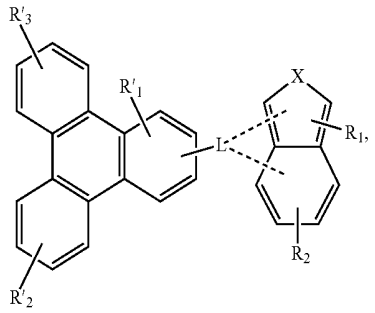
12. A first device comprising an organic light emitting device, further comprising:

an anode;

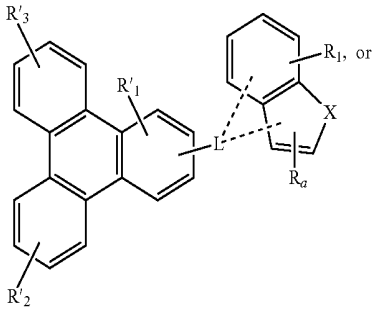
a cathode; and

an organic layer, disposed between the anode and the cathode, wherein the organic layer comprises a compound comprising one of the formulae:

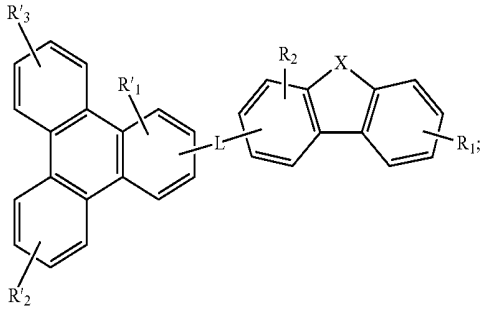
Formula 2



Formula 3



Formula 4



wherein X is S or Se;

wherein R_1, R_2, and R_a are independently selected from hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl;

wherein each of R_1 and R_2 may represent mono, di, tri or tetra substituents;

wherein at least two substituents of R_1 or R_2 are joined to form a fused ring;

wherein R_a represents mono or di substituents which cannot fuse to form a benzo ring; and

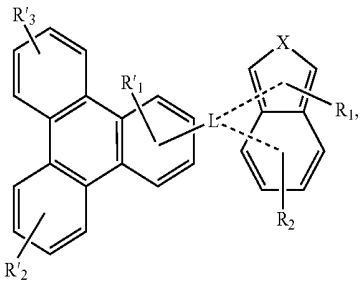
wherein L represents a spacer or a direct connection to the benzothiophene, or benzoselenophene moiety with additional fused rings;

wherein R'_1, R'_2, and R'_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl;

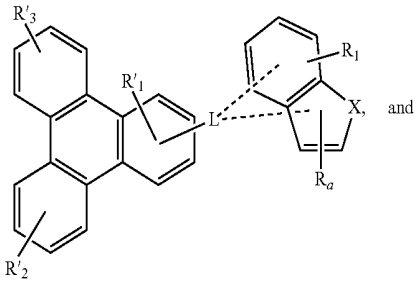
wherein each of R'_1, R'_2 and R'_3 may represent mono, di, tri, or tetra substituents.

13. The first device of claim **12**, wherein the compound is selected from the group consisting of:

Formula 2

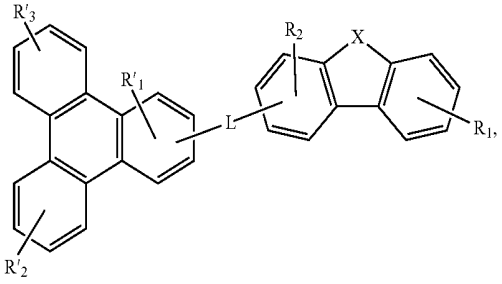


Formula 3



and

Formula 4



wherein X is S or Se;

wherein R_1, R_2, and R_a are independently selected from hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl;

wherein each of R_1 and R_2 may represent mono, di, tri or tetra substituents;

wherein at least two substituents of R_1 or R_2 are joined to form a fused ring;

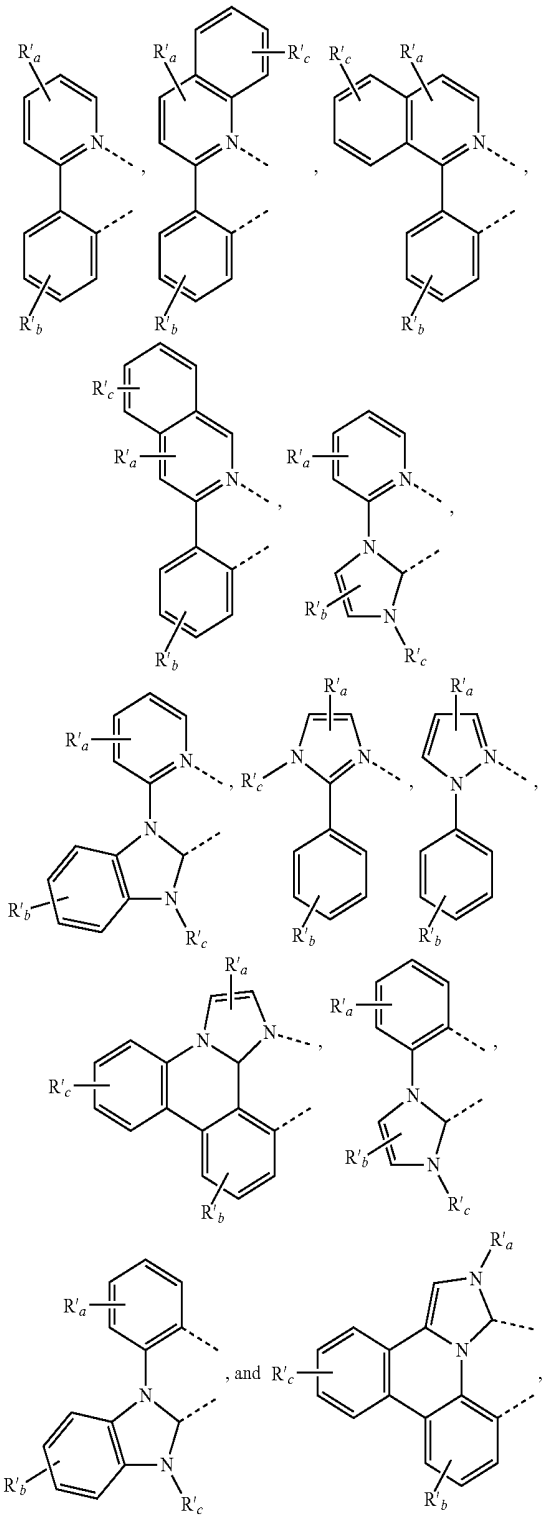
wherein R_a represents mono or di substituents which cannot fuse to form a benzo ring; and

wherein L represents a spacer or a direct connection to the benzothiophene, or benzoselenophene moiety with additional fused rings.

14. The first device of claim **12**, wherein the organic layer is an emissive layer and the compound comprising one of Formulae 2-4 is the host.

15. The first device of claim **14**, wherein the organic layer further comprises an emissive compound.

16. The first device of claim **15**, wherein the emissive compound is a transition metal complex having at least one ligand selected from the group consisting of:



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

wherein each of R'_a, R'_b and R'_c substituent are independently selected from a group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, or heteroaryl; and wherein two adjacent substituents may form into a ring.

17. The first device of claim **12**, wherein the device comprises a second organic layer that is non-emissive, and the compound comprising Formula I is a non-emissive material in the second organic layer.

18. The first device of claim **12**, wherein the first device is an organic light emitting device.

19. The first device of claim **12**, wherein the first device is a consumer product.

* * * * *

UNITED STATES PATENT AND TRADEMARK OFFICE

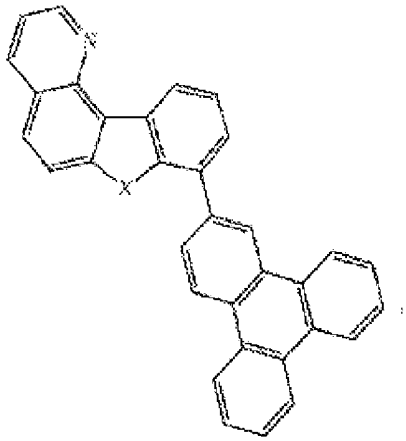
CERTIFICATE OF CORRECTION

PATENT NO. : 8,968,887 B2
APPLICATION NO. : 13/004523
DATED : March 3, 2015
INVENTOR(S) : Bin Ma et al.

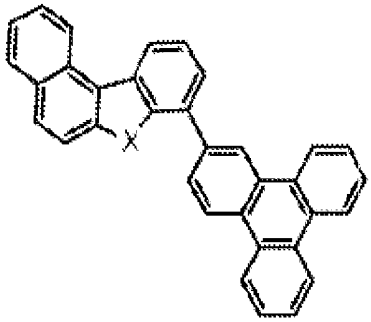
It is certified that error appears in the above-identified patent and that said Letters Patent is hereby corrected as shown below:

In the Specification

Compound 31



Column 29, Lines 36-53 – delete "



"

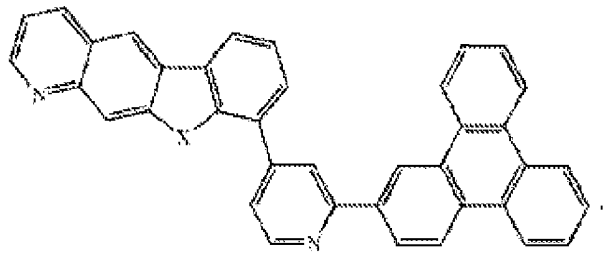
and insert -- Compound 33 --

Signed and Sealed this
Twenty-eighth Day of February, 2017

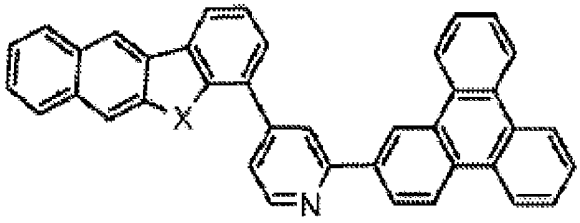
Michelle K. Lee

Michelle K. Lee
Director of the United States Patent and Trademark Office

Compound 34



Column 29, Lines 56-66 – delete "



Compound 34

and insert --

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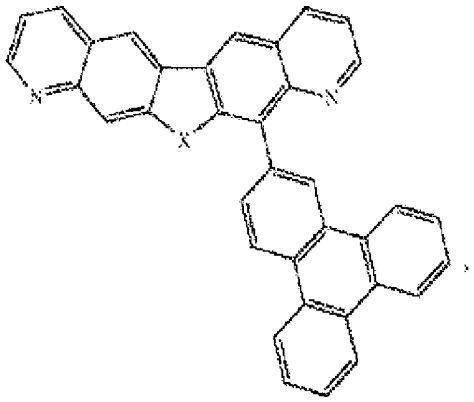
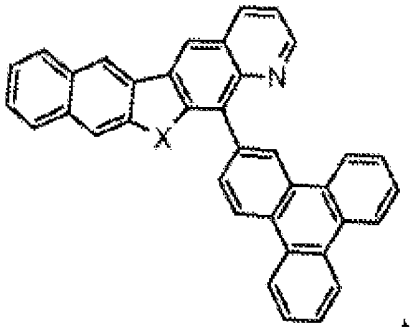
Compound 35



Column 30, Lines 5-19 – delete "

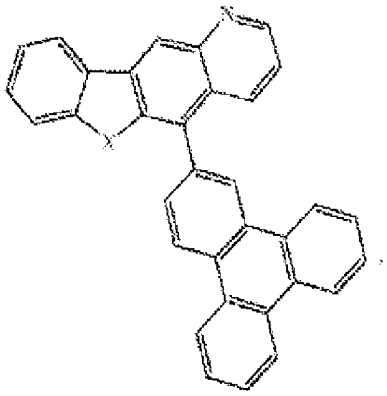


Compound 35

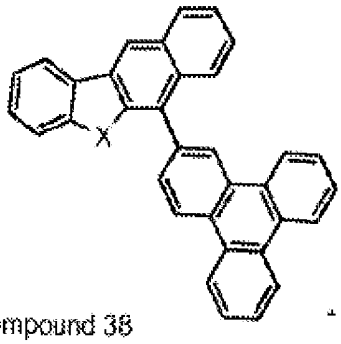
and insert --

--

Compound 38



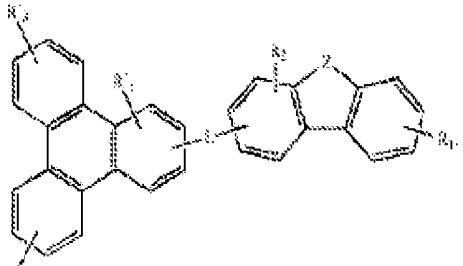
Column 30, Lines 53-66 – delete “ ”



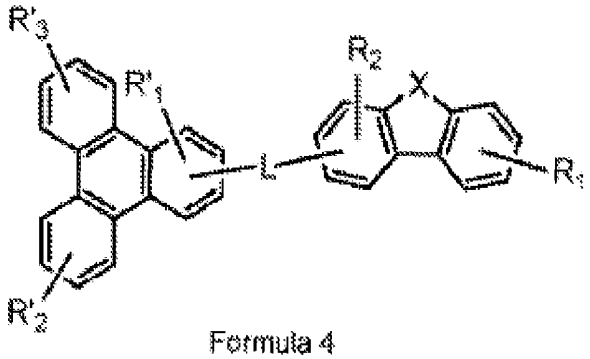
and insert -- Compound 38 --

In the Claims

Formula 4



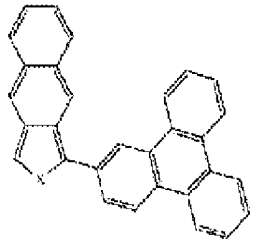
Claim 4, Column 123, Lines 4-14 – delete “ ”



Formula 4

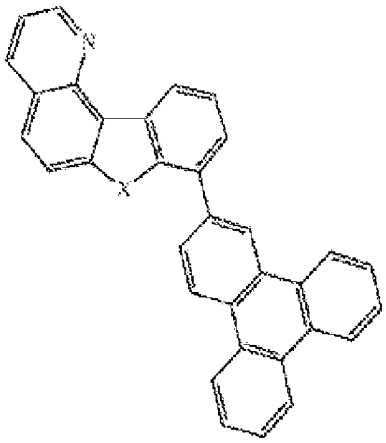
and insert -- --

Claim 11, Column 132, Lines 1-12 – delete "



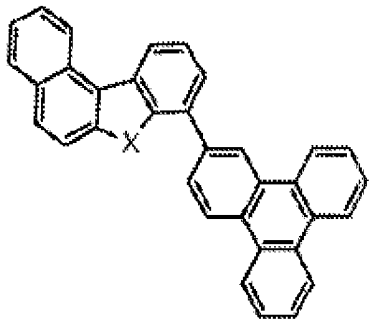
"

Claim 11, Column 138, Lines 1-18 – delete "

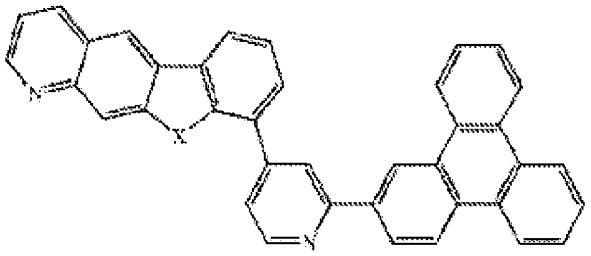


"

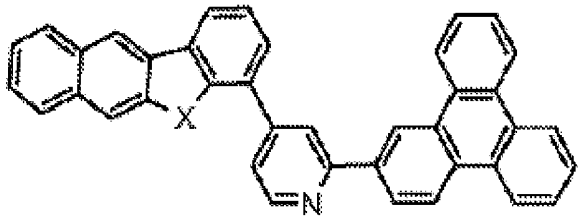
and insert -- Compound 33 --



Claim 11, Column 138, Lines 22-31 – delete "



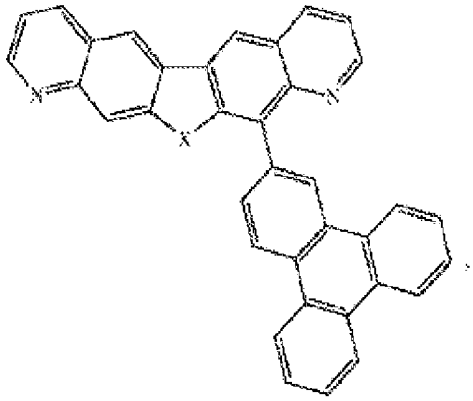
"



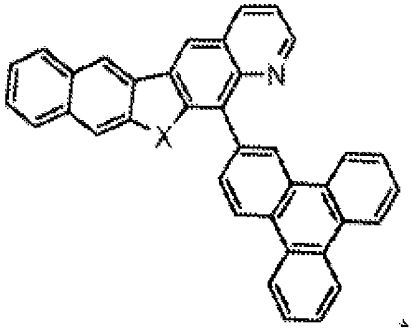
Compound 34

and insert -- Compound 34 --

Compound 35

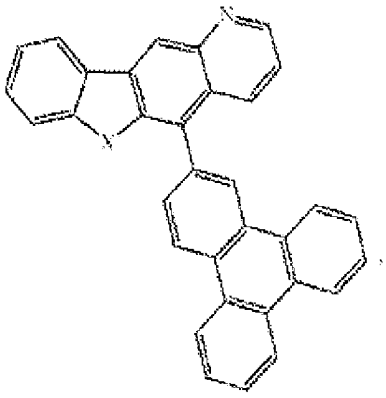


Claim 11, Column 138, Lines 34-48 – delete " "

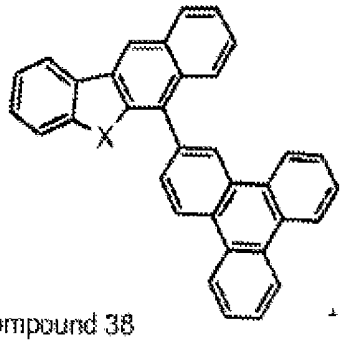


and insert -- Compound 35 --

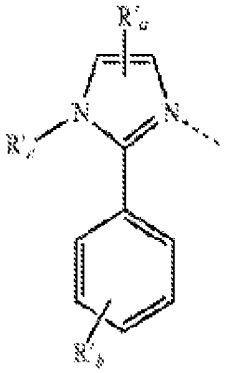
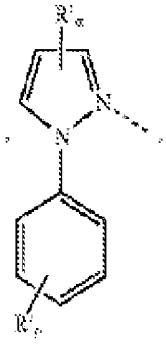
Compound 38

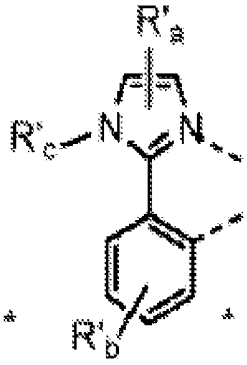


Claim 11, Column 139, Lines 17-31 – delete " "



and insert -- Compound 38 --

Claim 16, Column 148, Lines 34-44 – delete “  ” and “  ”

and insert --  -- and --  --

专利名称(译)	三亚苯 - 苯并呋喃/苯并噻吩/苯并硒吩化合物，其取代基连接形成稠合环		
公开(公告)号	US8968887	公开(公告)日	2015-03-03
申请号	US13/004523	申请日	2011-01-11
[标]申请(专利权)人(译)	环球展览公司		
申请(专利权)人(译)	通用显示器公司		
当前申请(专利权)人(译)	通用显示器公司		
[标]发明人	MA BIN FIORDELISO JAMES WU YONGGANG KWONG RAYMOND		
发明人	MA, BIN FIORDELISO, JAMES WU, YONGGANG KWONG, RAYMOND		
IPC分类号	H01L51/54 C07D307/77 C07D333/50 C09K11/06 H01L51/00 H01L51/50 H05B33/20 H05B33/22		
CPC分类号	C09K11/06 H01L51/0054 H05B33/20 H05B33/22 C09K2211/1088 C09K2211/1092 C09K2211/1096 H01L51/0072 H01L51/0074 H01L51/5012 C07D333/50 C07D345/00 C09K2211/1007 C09K2211/1011 H01L51/0071 H01L51/50		
代理机构(译)	DUANE MORRIS LLP		
优先权	61/343402 2010-04-28 US		
其他公开文献	US20110266526A1		
外部链接	Espacenet USPTO		

摘要(译)

提供了包含三亚苯基部分和苯并 - 或二苯并 - 部分的化合物。特别地，苯并 - 或二苯并 - 部分具有稠合的取代基。这些化合物可用于有机发光器件中，特别是与黄色，橙色和红色发光体组合使用，以提供具有改进性能的器件。