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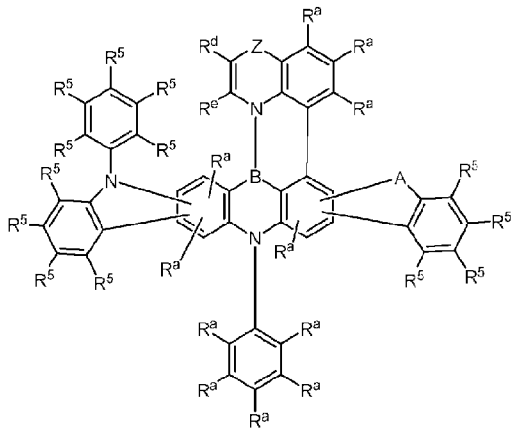
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(54) Title: ORGANIC MOLECULES FOR OPTOELECTRONIC DEVICES

(57) Abstract: The invention relates to an organic molecule, in particular for the use in optoelectronic devices. According to the invention, the organic molecule has a structure of formula I, wherein R^a, R^d and R^e is independently selected from the group consisting of: hydrogen, deuterium, $N(R^a)_2$, OR^a, $Si(R^a)_3$, $B(OR^a)_2$, $B(R^a)_2$,OSO_2R^a, CF_3, CN, F, Cl, Br, I, C_1-C_{40}-alkyl, C_1-C_{40}-alkoxy, C_1-C_{40}-thioalkoxy, C_2-C_{40}-alkenyl, C_2-C_{40}-alkynyl, C_6-C_{60}-aryl, and C_2-C_{57}-heteroaryl.



Formula I

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Description

Title of Invention: ORGANIC MOLECULES FOR OPTO-ELECTRONIC DEVICES

Technical Field

[1] The invention relates to light-emitting organic molecules and their use in organic light-emitting diodes (OLEDs) and in other optoelectronic devices.

Disclosure of Invention

Technical Problem

[2] The object of the present invention is to provide molecules which are suitable for use in optoelectronic devices.

Solution to Problem

[3] This object is achieved by the invention which provides a new class of organic molecules.

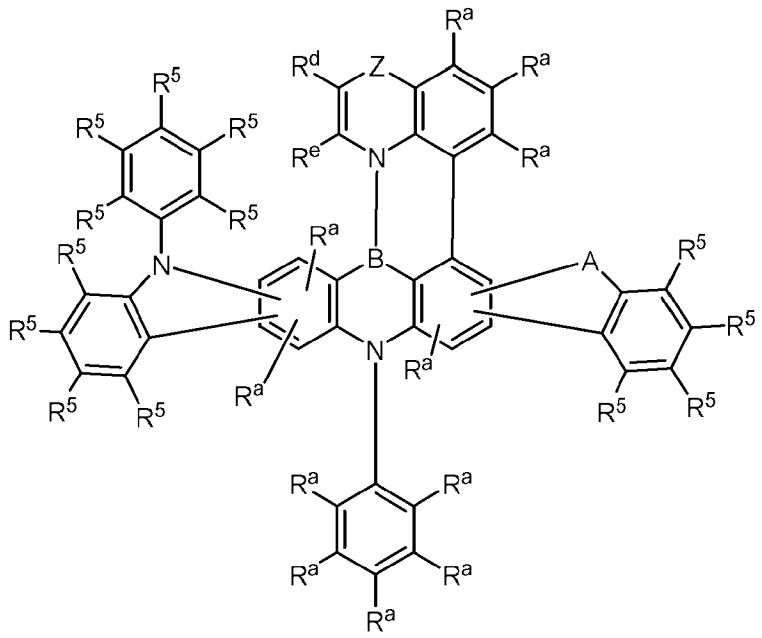
[4] According to the invention the organic molecules are purely organic molecules, i.e. they do not contain any metal ions in contrast to metal complexes known for use in optoelectronic devices.

[5] According to the present invention, the organic molecules exhibit emission maxima in the blue or sky-blue spectral range. The organic molecules exhibit in particular emission maxima below 560 nm, more preferably below 550 nm, even more preferably below 545 nm or even below 540 nm. It will typically be above 500 nm, more preferably above 510 nm, even more preferably above 515 nm or even above 520 nm. The photoluminescence quantum yields of the organic molecules according to the invention are, in particular, 50 % or more. The use of the molecules according to the invention in an optoelectronic device, for example an organic light-emitting diode (OLED), leads to higher efficiencies or higher color purity, expressed by the full width at half maximum (FWHM) of emission, of the device. Corresponding OLEDs have a higher stability than OLEDs with known emitter materials and comparable color. In particular, the molecules can be used in combination with thermally activated delayed fluorescence (TADF) materials and/or phosphorescence materials to enable so-called hyperfluorescence and/or hyperphosphorescence, respectively.

[6] Organic molecules according to the invention

[7] The organic light-emitting molecule of the invention comprises or consists of a structure of formula I

[8]



[9] Formula I

[10] wherein

[11] Z is at each occurrence independently selected from the group consisting of a direct bond, CR^3R^4, $C=CR^3R^4$, C=O, $C=NR^3$, NR^3, O, SiR^3R^4, S, S(O) and $S(O)_2$;

[12] A is selected from the group consisting of O, S, and NR^5;

[13] R^d and R^e is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^a)_2$, OR^a, $Si(R^a)_3$, $B(OR^a)_2$, $B(R^a)_2$, OSO_2R^a, CF_3, CN, F, Cl, Br, I,

[14] C_1-C_{40}-alkyl,

[15] which is optionally substituted with one or more substituents R^a and

[16] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

[17] C_1-C_{40}-alkoxy,

[18] which is optionally substituted with one or more substituents R^a and

[19] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

[20] C_1-C_{40}-thioalkoxy,

[21] which is optionally substituted with one or more substituents R^a and

[22] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

[23] C_2-C_{40}-alkenyl,

[24] which is optionally substituted with one or more substituents R^a and

[25] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

[26] C_2-C_{40}-alkynyl,

[27] which is optionally substituted with one or more substituents R^a and

[28] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

[29] C_6-C_{60}-aryl,

[30] which is optionally substituted with one or more substituents R^a; and

[31] C_2-C_{57}-heteroaryl,

[32] which is optionally substituted with one or more substituents R^a;

[33] R^a, R^3 and R^4 is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^5)_2$, OR^5, $Si(R^5)_3$, $B(OR^5)_2$, $B(R^5)_2$, OSO_2R^5, CF_3, CN, F, Cl, Br, I,

[34] C_1-C_{40}-alkyl,

[35] which is optionally substituted with one or more substituents R^5 and

[36] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[37] C_1-C_{40}-alkoxy,

[38] which is optionally substituted with one or more substituents R^5 and

[39] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[40] C_1-C_{40}-thioalkoxy,

[41] which is optionally substituted with one or more substituents R^5 and

[42] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[43] C_2-C_{40}-alkenyl,

[44] which is optionally substituted with one or more substituents R^5 and

[45] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[46] C_2-C_{40}-alkynyl,

[47] which is optionally substituted with one or more substituents R^5 and

[48] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[49] C_6-C_{60}-aryl,

[50] which is optionally substituted with one or more substituents R^5; and

[51] C_2-C_{57}-heteroaryl,

[52] which is optionally substituted with one or more substituents R^5;

[53] R^5 is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^6)_2$, OR^6, $Si(R^6)_3$, $B(OR^6)_2$, $B(R^6)_2$, OSO_2R^6, CF_3, CN, F, Br, I,

[54] C_1-C_{40}-alkyl,

[55] which is optionally substituted with one or more substituents R^6 and

[56] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[57] C_1-C_{40}-alkoxy,

[58] which is optionally substituted with one or more substituents R^6 and

[59] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[60] C_1-C_{40}-thioalkoxy,

[61] which is optionally substituted with one or more substituents R^6 and

[62] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[63] C_2-C_{40}-alkenyl,

[64] which is optionally substituted with one or more substituents R^6 and

[65] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[66] C_2-C_{40}-alkynyl,

[67] which is optionally substituted with one or more substituents R^6 and

[68] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[69] C_6-C_{60}-aryl,

[70] which is optionally substituted with one or more substituents R^6; and

[71] C_2-C_{57}-heteroaryl,

[72] which is optionally substituted with one or more substituents R^6;

[73] R^6 is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, OPh, CF_3, CN, F,

[74] C_1-C_5-alkyl,

[75] wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;

[76] C_1-C_5-alkoxy,

[77] wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;

[78] C_1-C_5-thioalkoxy,

[79] wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;

[80] C_2-C_5-alkenyl,

[81] wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;

[82] C_2-C_5-alkynyl,

[83] wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;

[84] C_6-C_{18}-aryl,

[85] which is optionally substituted with one or more C_1-C_5-alkyl substituents;

[86] C_2-C_{17}-heteroaryl,

[87] which is optionally substituted with one or more C_1-C_5-alkyl substituents;

[88] $N(C_6\text{-}C_{18}\text{-aryl})_2$;

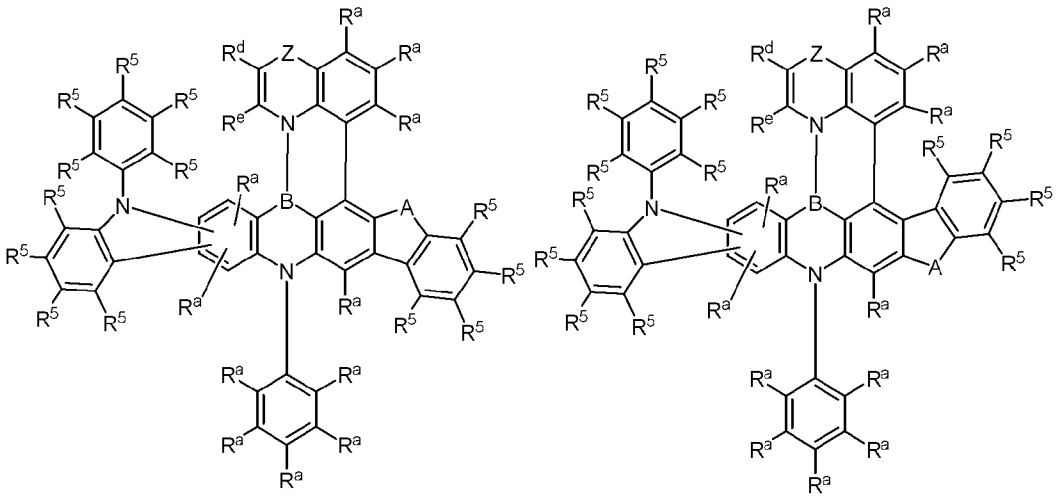
[89] $N(C_2\text{-}C_{17}\text{-heteroaryl})_2$, and

[90] $N(C_2\text{-}C_{17}\text{-heteroaryl})(C_6\text{-}C_{18}\text{-aryl})$;

[91] wherein any of the substituents R^a, R^3, R^4, R^d, R^e, R^5, and R^6 optionally independently form a mono- or polycyclic, aliphatic, aromatic, heteroaromatic and/or benzo-fused ring system with one or more substituents R^a, R^3, R^4, R^d, R^e, R^5 and/or R^6.

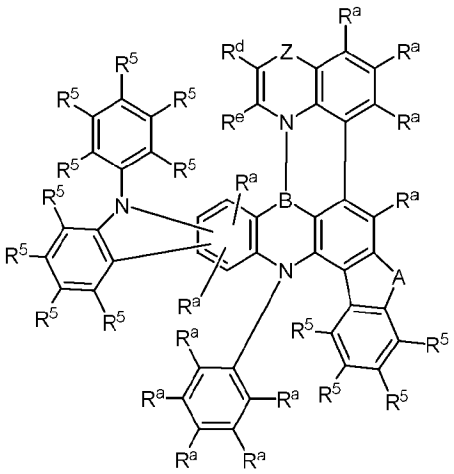
[92] Exemplary embodiments of organic molecules according to Formula I are provided in the following:

[93]



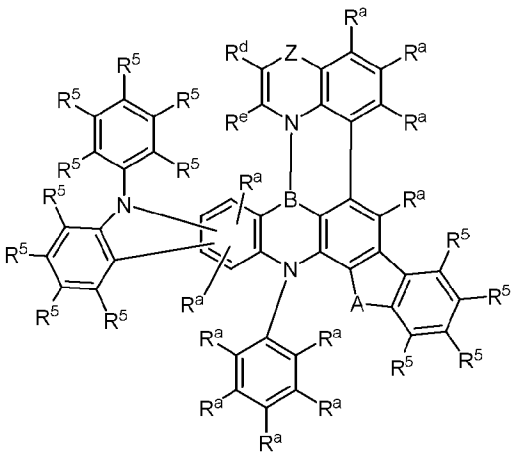
[94] Formula I-1 Formula I-2

[95]



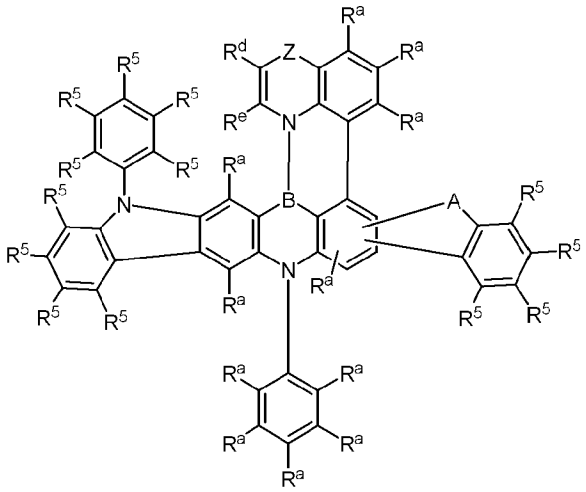
[96] Formula I-3

[97]



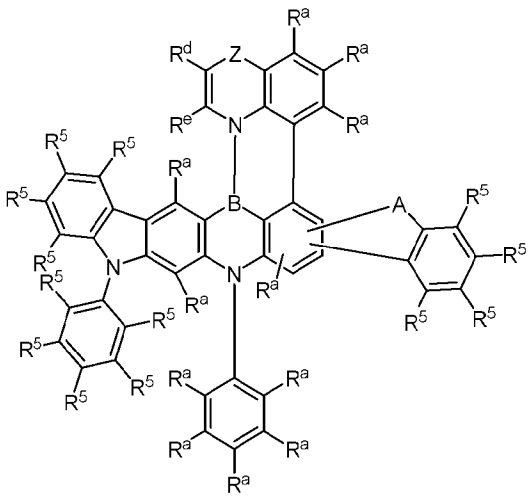
[98] Formula I-4

[99]



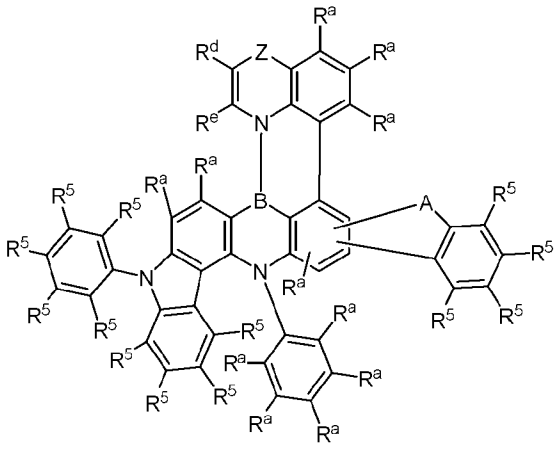
[100] Formula I-5

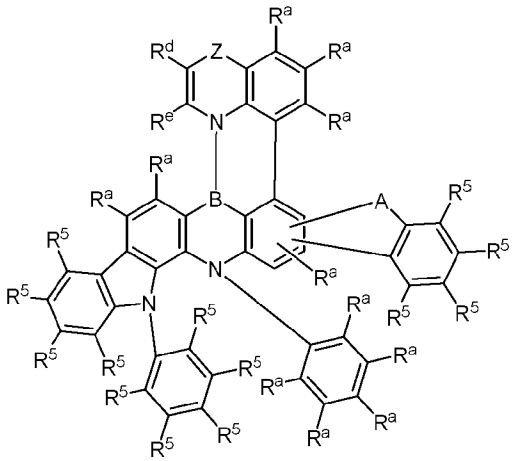
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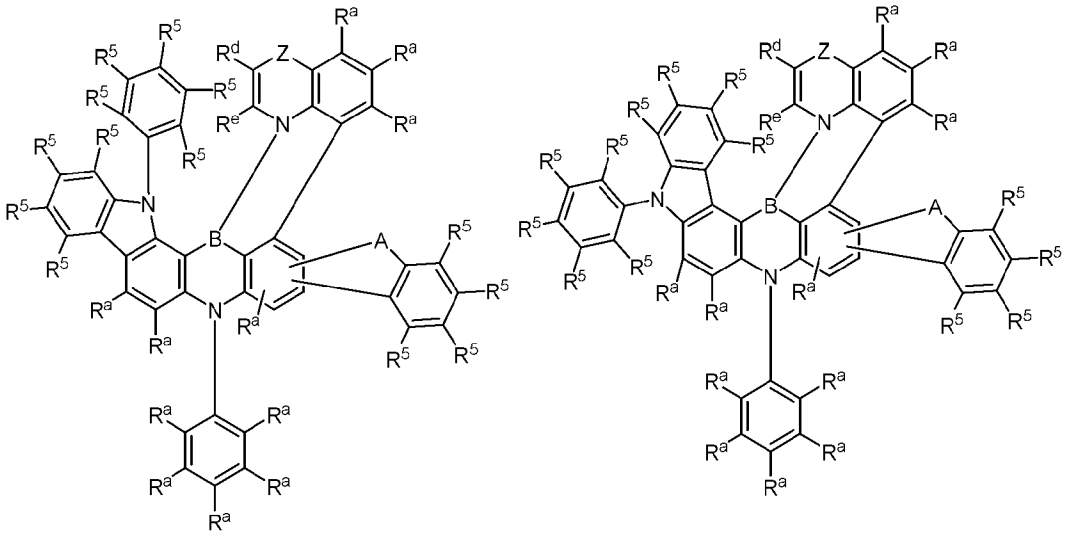
[102] Formula I-6

[103]





[104] Formula I-7 Formula I-8

[105] 

[106] Formula I-9 Formula I-10.

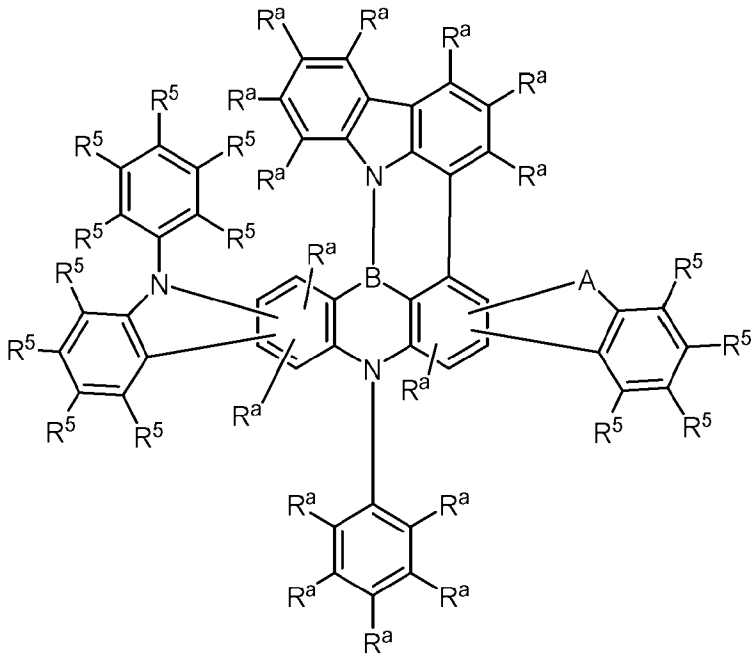
[107] In one embodiment, Z is selected from the group consisting of a direct bond, C=O, and NR^3.

[108] In a preferred embodiment, Z is a direct bond.

[109] In a preferred embodiment, A is O.

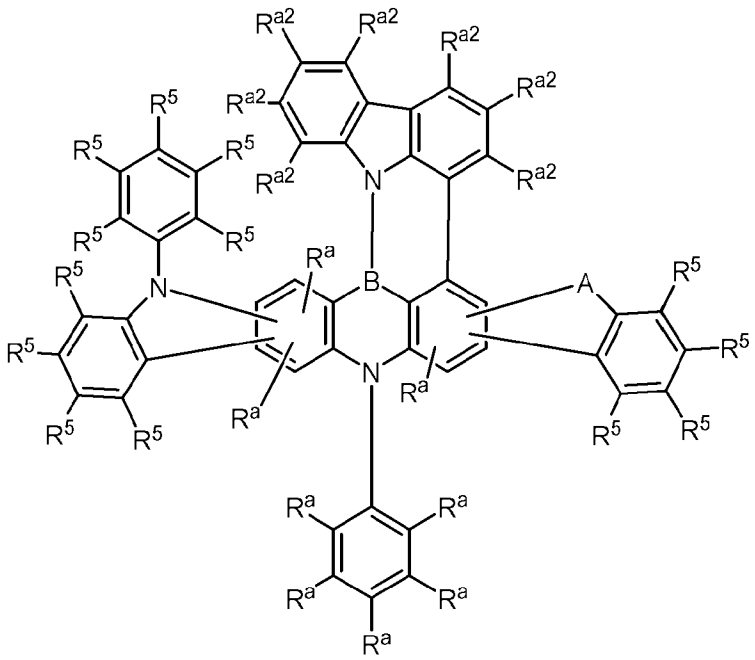
[110] In one embodiment, R^d and R^e are hydrogen.

[111] In one embodiment, the organic molecules comprise or consist of a structure of formula Ia:

[112] 

[113] Formula Ia.

[114] In one embodiment, the organic molecules comprise or consist of a structure of formula Ia-2:

[115] 

[116] Formula Ia-2,

[117] wherein R^{a2} is at each occurrence independently from another selected from the group consisting of:

[118] hydrogen,

[119] deuterium,

[120] Me,

[121] ^{i}Pr,

[122] ^{t}Bu,

[123] CN,

[124] CF_3,

[125] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[126] pyridinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

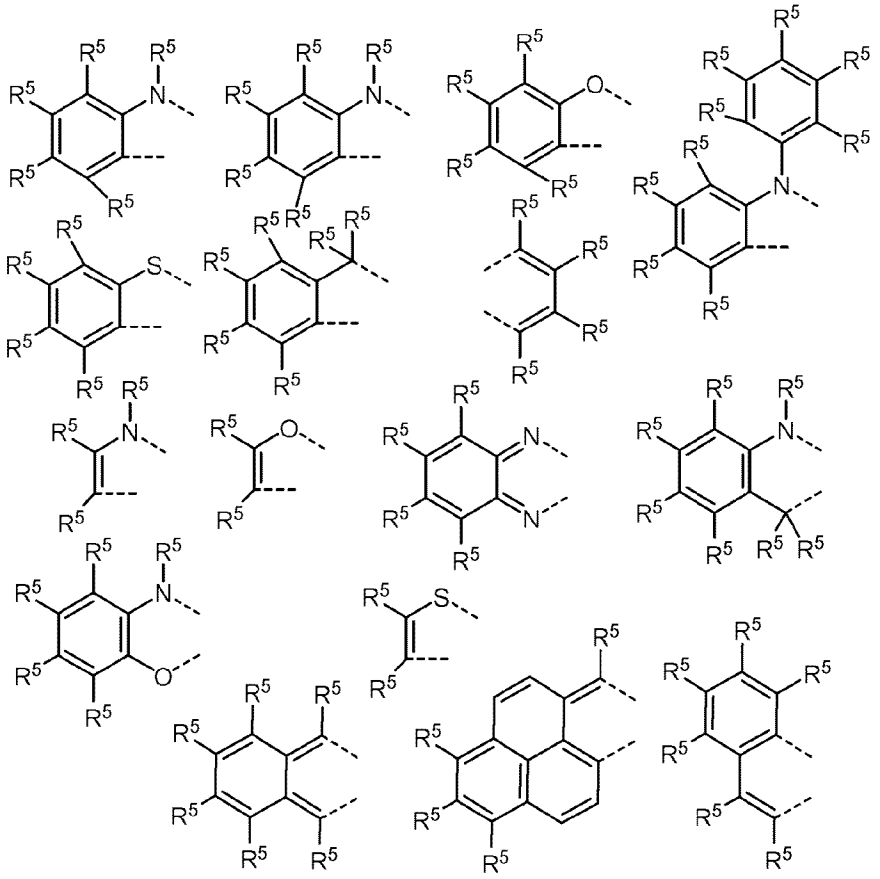
[127] pyrimidinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[128] carbazolyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[129] triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[130] and $N(Ph)_2$, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph;

[131] wherein two or more adjacent substituents R^a may form attachment points for a ring system selected from the group consisting of:

[132] 

[133] wherein each dashed line indicates a direct bond connecting one of the above shown ring systems to the positions of two adjacent substituents R^{a2} such that a ring system of the group shown above is fused to the structure as shown in Formula Ia-2.

[134] In a further embodiment of the invention, R^{a2} is at each occurrence independently from another selected from the group consisting of:

[135] hydrogen,

[136] Me,

[137] ^{i}Pr,

[138] ^{t}Bu,

[139] CN,

[140] CF_3,

[141] Ph, which is optionally substituted with one or more substituents R^5,

[142] pyridinyl, which is optionally substituted with one or more substituents R^5,

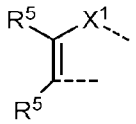
[143] pyrimidinyl, which is optionally substituted with one or more substituents R^5,

[144] carbazolyl, which is optionally substituted with one or more substituents R^5,

[145] triazinyl, which is optionally substituted with one or more substituents R^5,

[146] and $N(Ph)_2$, which is optionally substituted with one or more substituents R^5;

[147] wherein any two of the groups R^a positioned adjacent to each other are optionally bonded to each other and form a ring system selected from a group consisting of:

[148] 

[149] wherein X^1 is S, O or NR^5.

[150] In a further embodiment of the invention, R^{a2} is at each occurrence independently from another selected from the group consisting of:

[151] hydrogen,

[152] Me,

[153] ^{i}Pr,

[154] ^{t}Bu,

[155] CN,

[156] CF_3,

[157] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[158] pyridinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[159] pyrimidinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph, and

[160] triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

[161] In a further embodiment of the invention, R^{a2} is at each occurrence independently from another selected from the group consisting of:

[162] hydrogen,

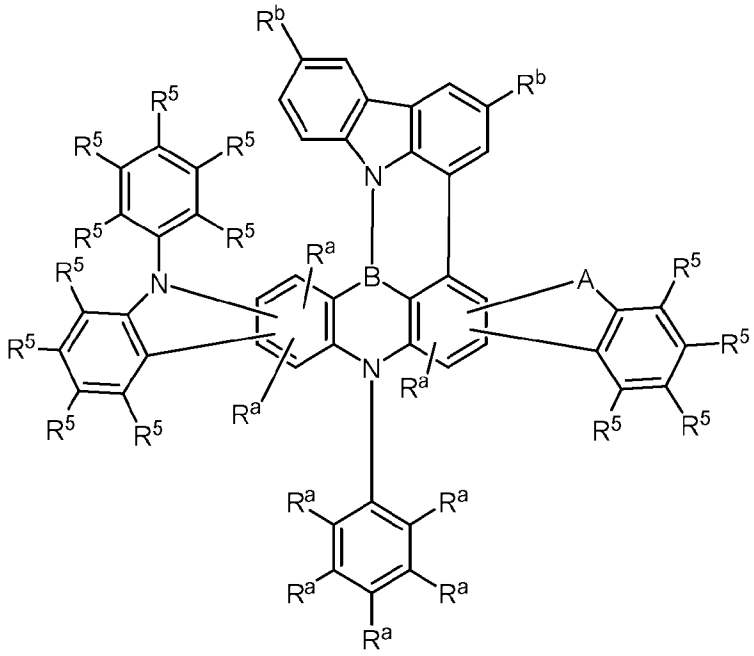
[163] Me,

[164] ^{i}Pr,

[165] ^{t}Bu,

[166] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

[167] In one embodiment, the organic molecules comprise or consist of a structure of formula Ib:

[168] 

[169] Formula Ib

[170] wherein R^b is at each occurrence independently from another selected from the group consisting of hydrogen, deuterium, $N(R^5)_2$, OR^5, $Si(R^5)_3$, $B(OR^5)_2$, OSO_2R^5, CF_3, CN, F, Br, I,

[171] C_1-C_{40}-alkyl,

[172] which is optionally substituted with one or more substituents R^5 and

[173] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[174] C_1-C_{40}-alkoxy,

[175] which is optionally substituted with one or more substituents R^5 and

[176] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[177] C_1-C_{40}-thioalkoxy,

[178] which is optionally substituted with one or more substituents R^5 and

[179] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[180] C_2-C_{40}-alkenyl,

[181] which is optionally substituted with one or more substituents R^5 and

[182] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[183] C_2-C_{40}-alkynyl,

[184] which is optionally substituted with one or more substituents R^5 and

[185] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C{=}CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C{=}NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

[186] C_6-C_{60}-aryl,

[187] which is optionally substituted with one or more substituents R^5; and

[188] C_2-C_{57}-heteroaryl,

[189] which is optionally substituted with one or more substituents R^5.

[190] In a further embodiment of the invention, R^b is at each occurrence independently from another selected from the group consisting of:

[191] hydrogen, deuterium,

[192] Me, ^{i}Pr, ^{t}Bu, CN, CF_3,

[193] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[194] pyridinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[195] carbazolyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[196] triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[197] and $N(Ph)_2$.

[198] In a further embodiment of the invention, R^b is at each occurrence independently from another selected from the group consisting of:

[199] Me, ^{i}Pr, ^{t}Bu, CN, CF_3,

[200] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

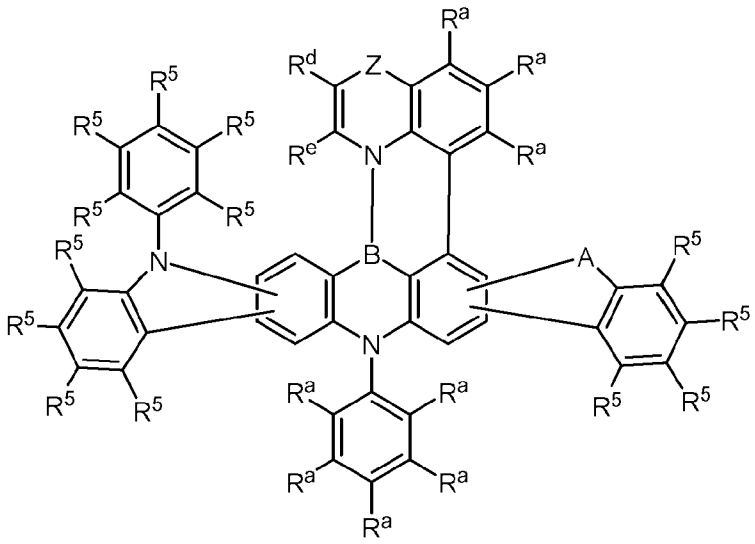
[201] pyridinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[202] carbazolyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

[203] triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

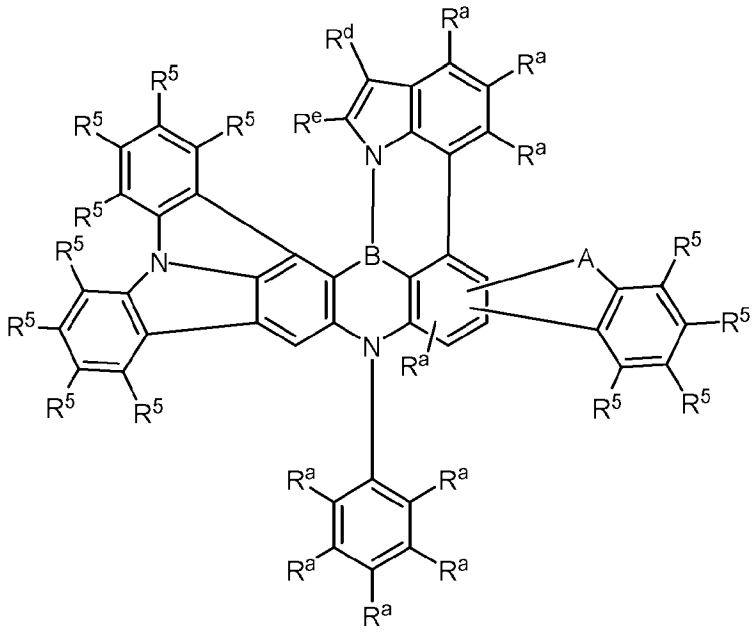
[204] and $N(Ph)_2$.

[205] In one embodiment, the organic molecules comprise or consist of a structure of formula II:

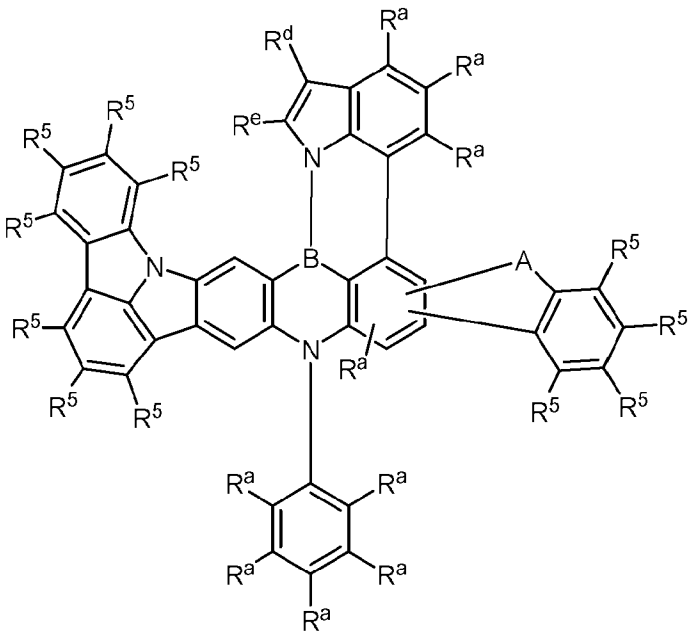
[206] 

[207] Formula II.

[208] In one embodiment, the organic molecules comprise or consist of a structure of formula IIa or formula IIb:

[209] 

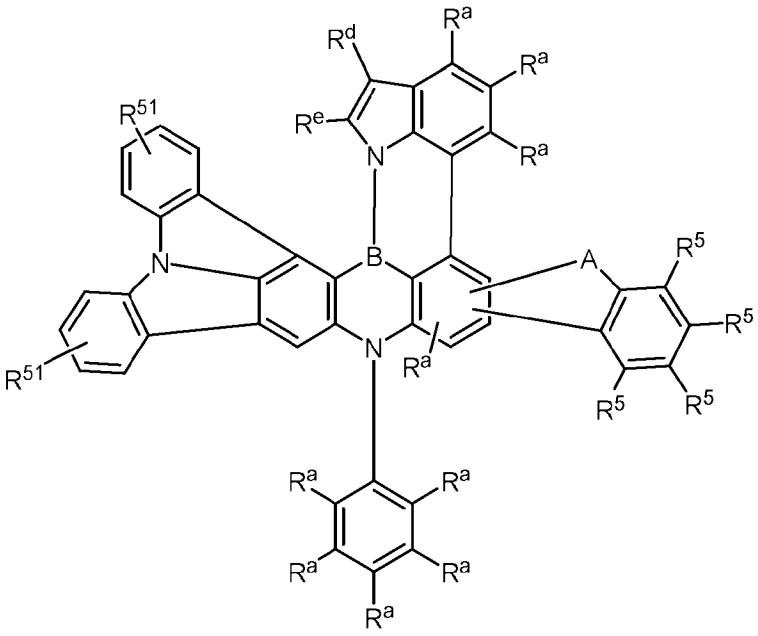
[210] Formula IIa,

[211] 

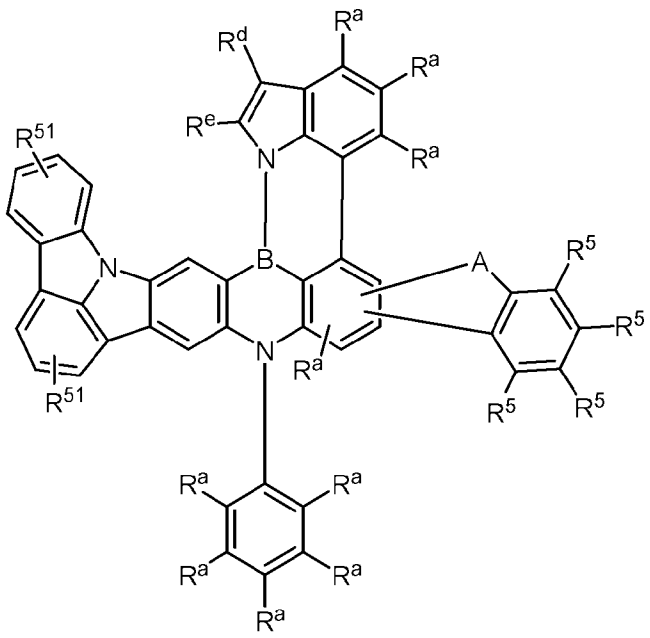
[212] Formula IIb.

[213] In a preferred embodiment, the organic molecules comprise or consist of a structure of formula IIa.

[214] In one embodiment, the organic molecules comprise or consist of a structure of formula IIa-2 or formula IIb-2:

[215] 

[216] Formula IIa-2,

[217] 

[218] Formula IIb-2,

[219] wherein R^{51} is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^6)_2$, OR^6, $Si(R^6)_3$, $B(OR^6)_2$, $B(R^6)_2$, OSO_2R^6, CF_3, CN, F, Br, I,

[220] C_1-C_{40}-alkyl,

[221] which is optionally substituted with one or more substituents R^6 and

[222] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[223] C_1-C_{40}-alkoxy,

[224] which is optionally substituted with one or more substituents R^6 and

[225] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[226] C_1-C_{40}-thioalkoxy,

[227] which is optionally substituted with one or more substituents R^6 and

[228] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[229] C_2-C_{40}-alkenyl,

[230] which is optionally substituted with one or more substituents R^6 and

[231] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[232] C_2-C_{40}-alkynyl,

[233] which is optionally substituted with one or more substituents R^6 and

[234] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, $C\equiv C$, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[235] C_6-C_{60}-aryl,

[236] which is optionally substituted with one or more substituents R^6; and

[237] C_2-C_{57}-heteroaryl,

[238] which is optionally substituted with one or more substituents R^6.

[239] In one embodiment, R^{51} is at each occurrence independently from another selected from the group consisting of:

[240] hydrogen,

[241] Me,

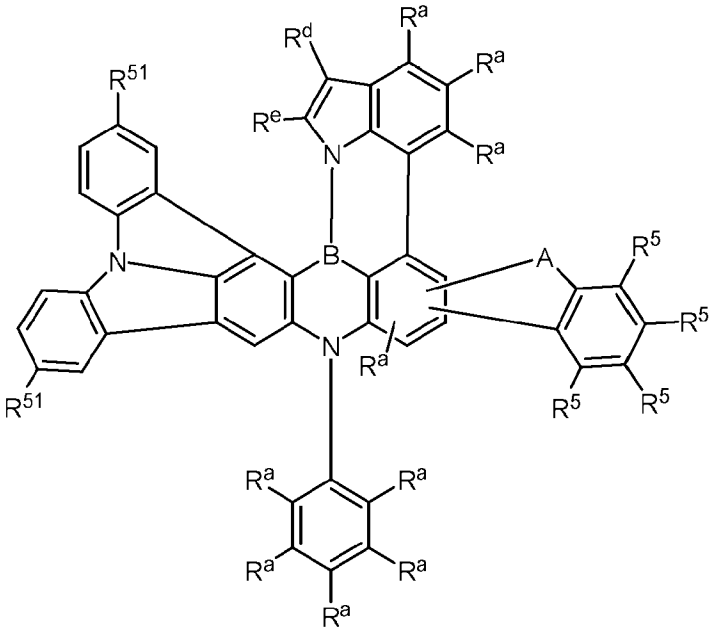
[242] ^{i}Pr,

[243] ^{t}Bu,

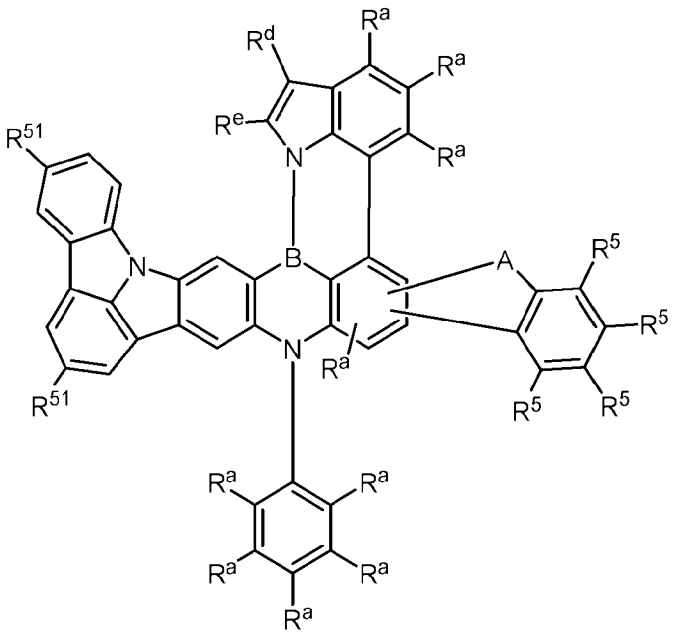
[244] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

[245] In one embodiment, the organic molecules comprise or consist of a structure of formula IIa-3 or formula IIb-3:

[246]



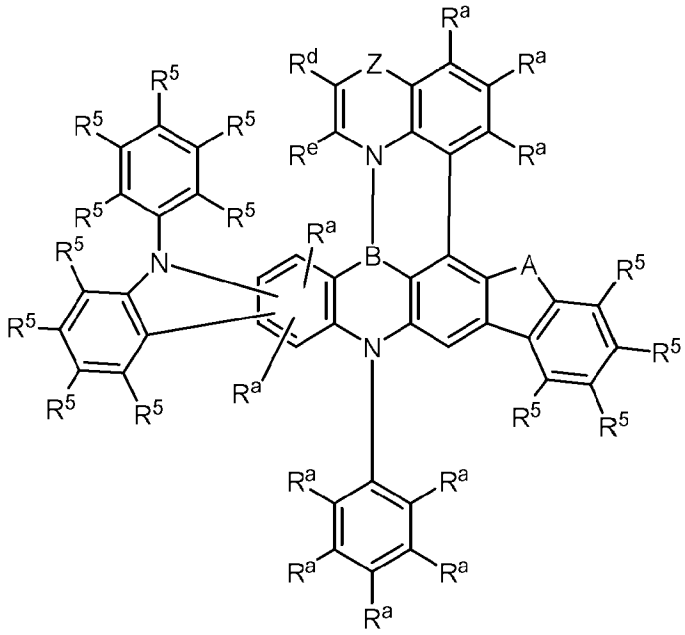
[247] Formula IIa-3,

[248] 

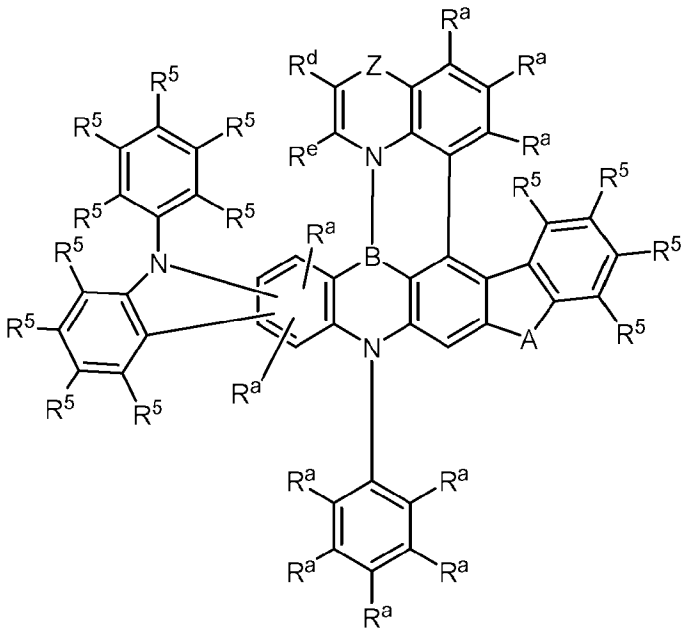
[249] Formula IIb-3.

[250] In one embodiment, R^{51} is at each occurrence hydrogen.

[251] In one embodiment, the organic molecules comprise or consist of a structure of formula IIIa or formula IIIb:

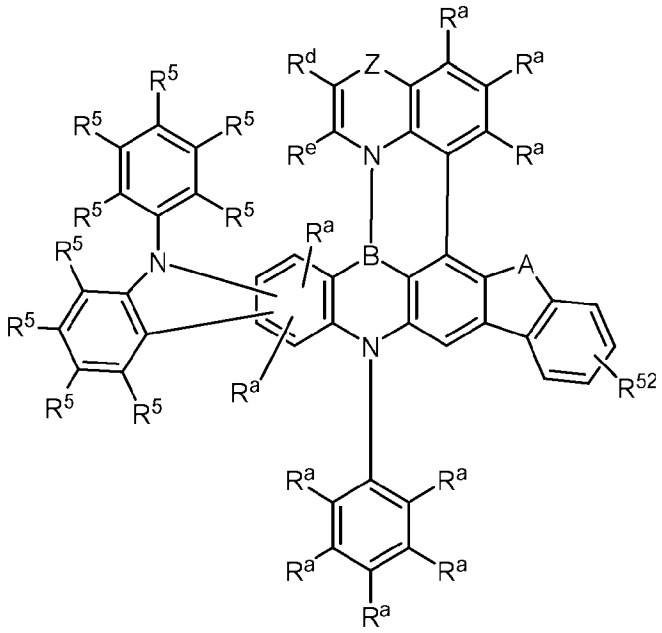
[252] 

[253] Formula IIIa,

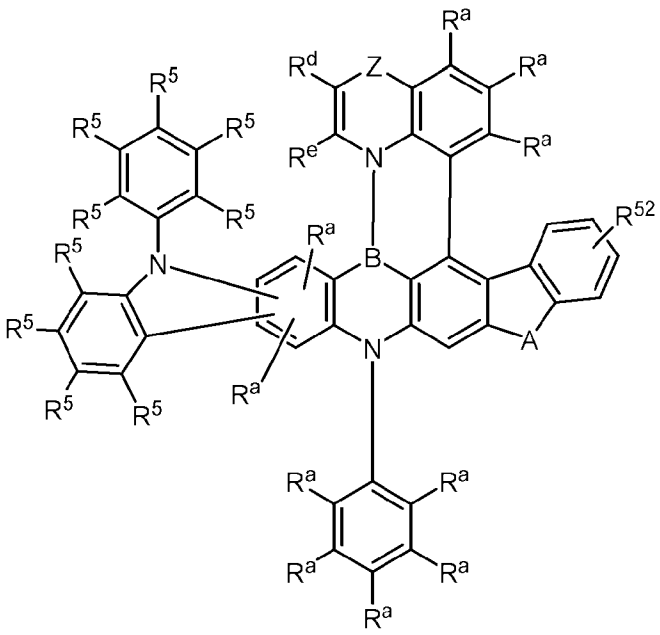
[254] 

[255] Formula IIIb.

[256] In one embodiment, the organic molecules comprise or consist of a structure of formula IIIa-2 or formula IIIb-2:

[257] 

[258] Formula IIIa-2,

[259] 

[260] Formula IIIb-2,

[261] wherein R^{52} is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^6)_2$, OR^6, $Si(R^6)_3$, $B(OR^6)_2$, $B(R^6)_2$, OSO_2R^6, CF_3, CN, F, Br, I,

[262] C_1-C_{40}-alkyl,

[263] which is optionally substituted with one or more substituents R^6 and

[264] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[265] C_1-C_{40}-alkoxy,

[266] which is optionally substituted with one or more substituents R^6 and

[267] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[268] C_1-C_{40}-thioalkoxy,

[269] which is optionally substituted with one or more substituents R^6 and

[270] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[271] C_2-C_{40}-alkenyl,

[272] which is optionally substituted with one or more substituents R^6 and

[273] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[274] C_2-C_{40}-alkynyl,

[275] which is optionally substituted with one or more substituents R^6 and

[276] wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, $C\equiv C$, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

[277] C_6-C_{60}-aryl,

[278] which is optionally substituted with one or more substituents R^6; and

[279] C_2-C_{57}-heteroaryl,

[280] which is optionally substituted with one or more substituents R^6.

[281] In one embodiment, R^{52} is at each occurrence independently from another selected from the group consisting of:

[282] hydrogen,

[283] Me,

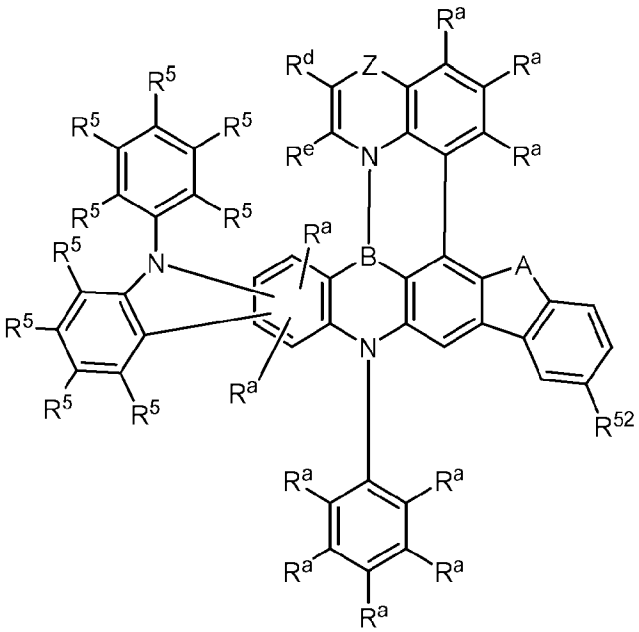
[284] ^{i}Pr,

[285] ^{t}Bu,

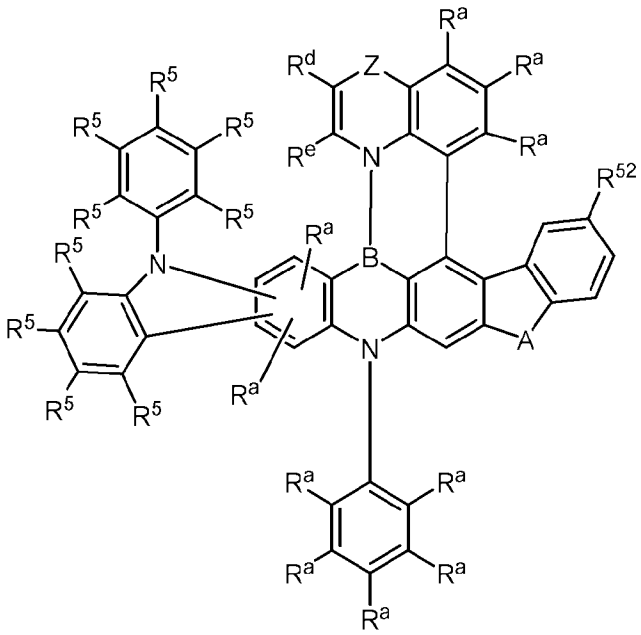
[286] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

[287] In one embodiment, the organic molecules comprise or consist of a structure of formula IIIa-3 or formula IIIb-3:

[288]



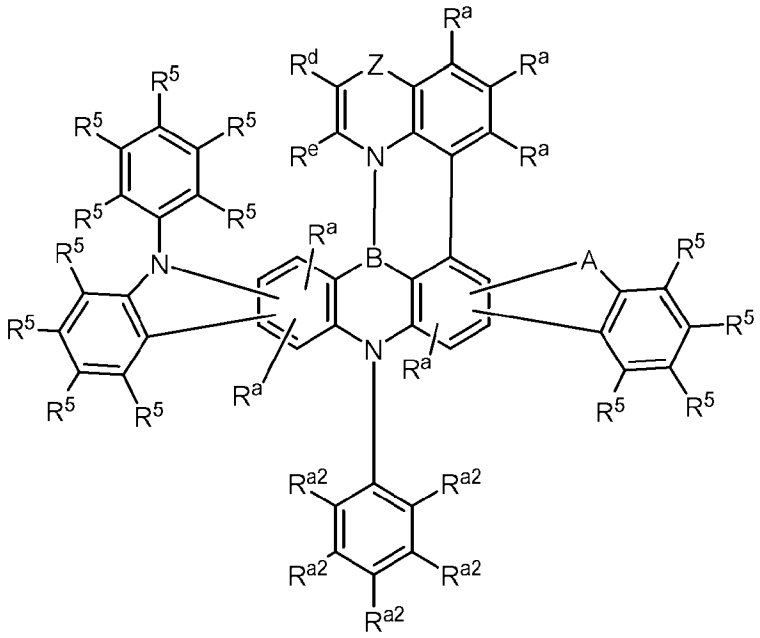
[289] Formula IIIa-3,

[290] 

[291] Formula IIIb-3.

[292] In one embodiment, R^{52} is at each occurrence hydrogen.

[293] In one embodiment, the organic molecules comprise or consist of a structure of formula IV:

[294] 

[295] Formula IV,

[296] wherein R^{a2} is at each occurrence independently from each other selected from R^a and any of the substituents R^a, R^5, and R^6 optionally independently form a mono- or polycyclic, aliphatic, aromatic, heteroaromatic and/or benzo-fused ring system with one or more substituents R^a, R^5 and/or R^6.

[297] In one embodiment, R^{a2} is at each occurrence independently from another selected

from the group consisting of:

[298] hydrogen,

[299] F,

[300] Me,

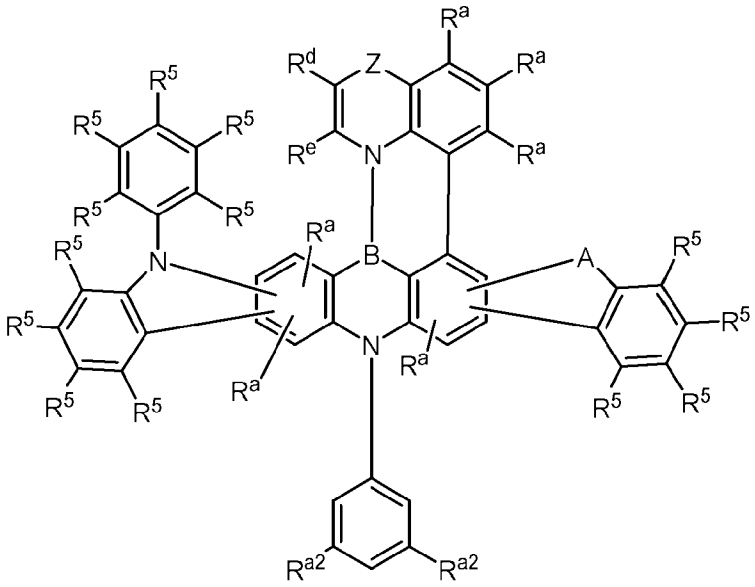
[301] ^{i}Pr,

[302] ^{t}Bu,

[303] Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

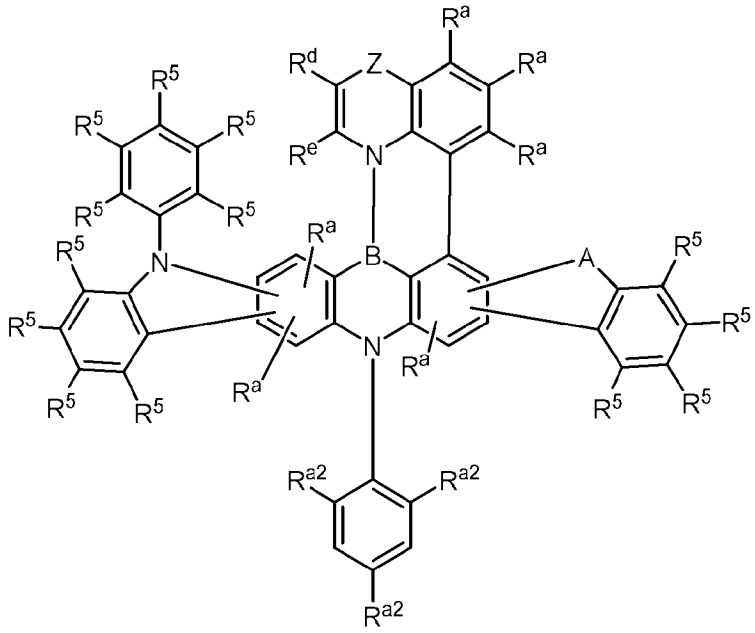
[304] In one embodiment, the organic molecules comprise or consist of a structure of formula IVa, formula IVb or formula IVc:

[305]



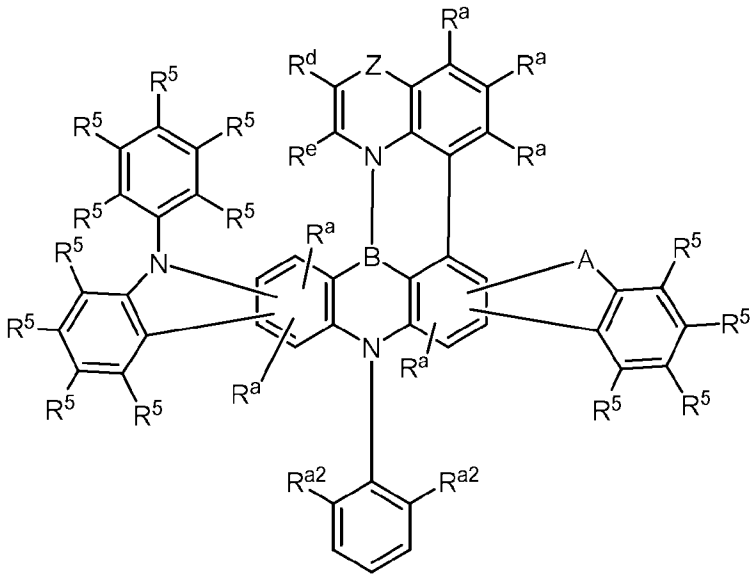
[306] Formula IVa,

[307]



[308] Formula IVb,

[309]



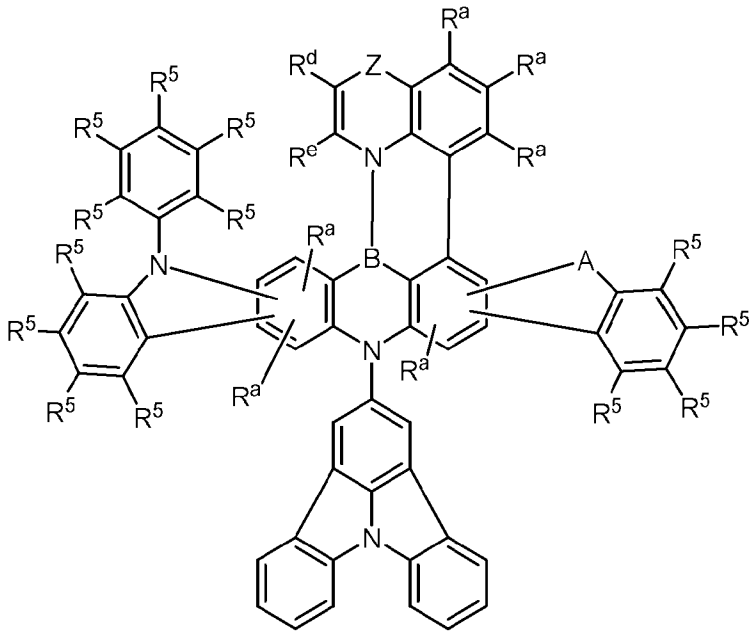
[310] Formula IVc.

[311] In one embodiment, the organic molecules comprise or consist of a structure of formula IV,

[312] wherein at least two of the substituents R^{a2}, preferably two adjacent substituents R^{a2}, form a mono- or polycyclic, aliphatic, aromatic, heteroaromatic and/or benzo-fused ring system.

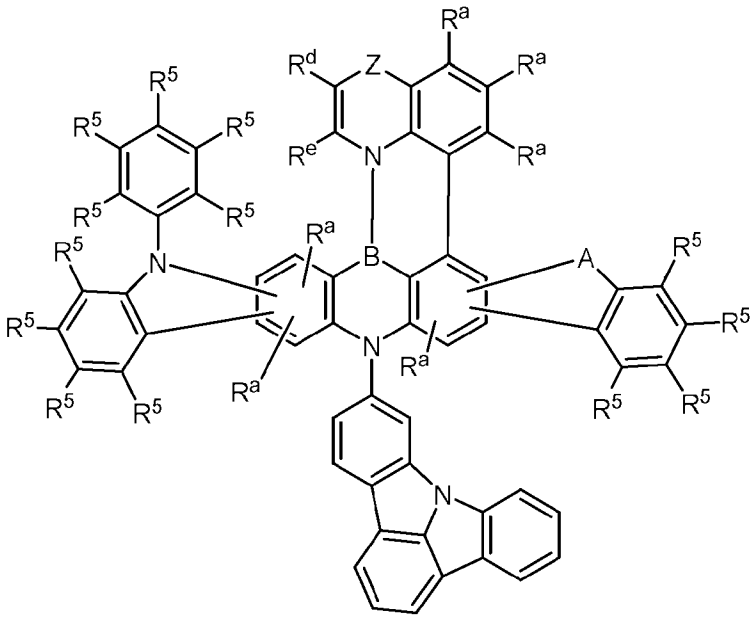
[313] In one embodiment, the organic molecules comprise or consist of a structure of formula IV-1, formula IV-2, formula IV-3, formula IV-4, and formula IV-5:

[314]



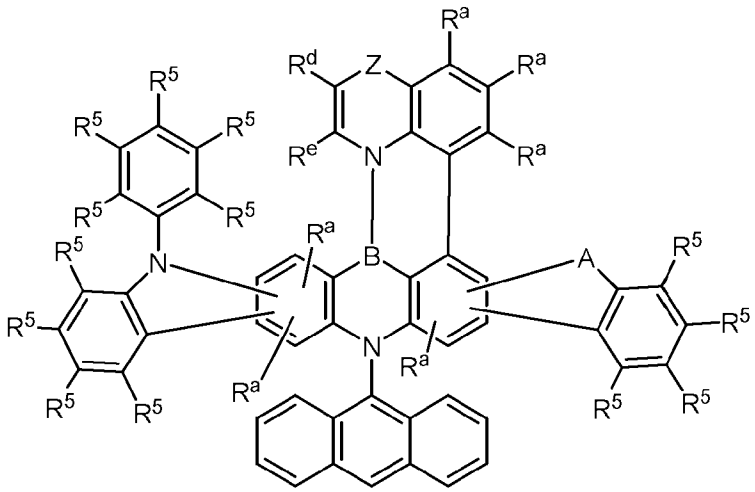
[315] Formula IV-1,

[316]



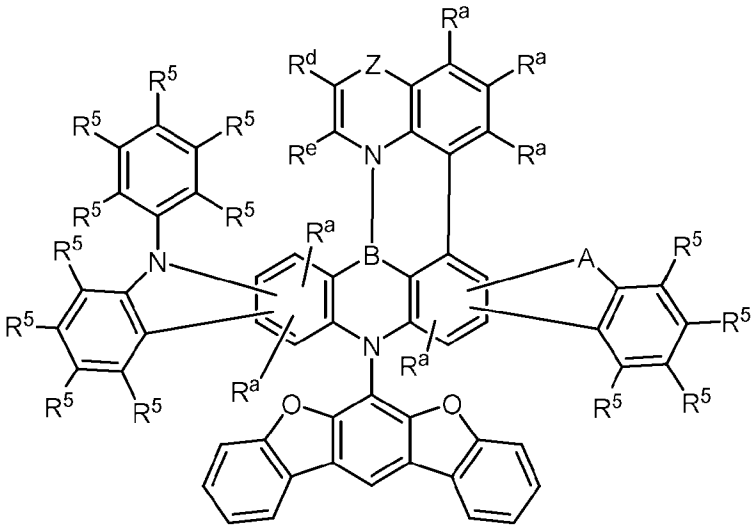
[317] Formula IV-2,

[318]

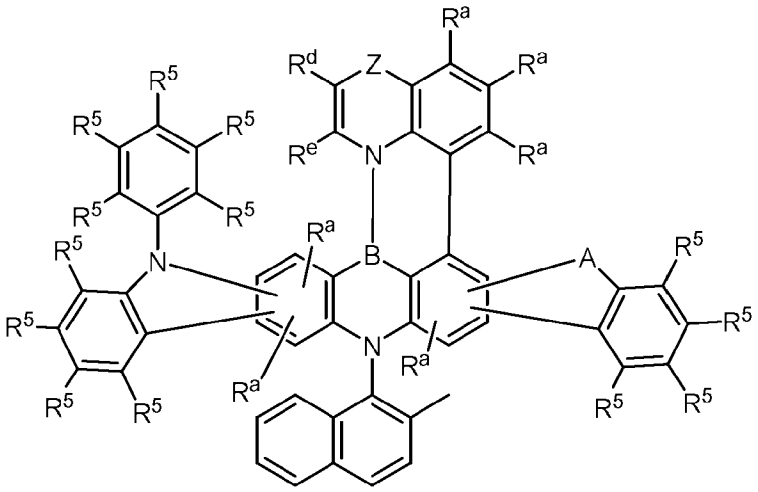


[319] Formula IV-3,

[320]



[321] Formula IV-4,

[322] 

[323] Formula IV-5.

[324] Definitions

[325] Herein, the term "layer" refers to a body that bears an extensively planar geometry. It forms part of the common knowledge of those skilled in that optoelectronic devices may be composed of several layers.

[326] A light-emitting layer (EML) in the context of the present invention is a layer of an optoelectronic device, wherein light emission from said layer is observed when applying a voltage and electrical current to the device. The person skilled in the art understands that light emission from optoelectronic devices is attributed to light emission from at least one EML. The skilled artisan understands that light emission from an EML is typically not (mainly) attributed to all materials comprised in said EML, to specific emitter materials.

[327] An "emitter material" (also referred to as "emitter") in the context of the present invention is a material that emits light when it is comprised in a light-emitting layer (EML) of an optoelectronic device (vide infra), given that a voltage and electrical current are applied to said device. The person skilled in the art knows that an emitter material usually is an "emissive dopant" material, and the skilled artisan understands that a dopant material (may it be emissive or not) is a material that is embedded in a matrix material that is usually (and herein) referred to as host material. Herein, host materials are also in general referred to as H^B when they are comprised in an optoelectronic device (preferably an OLED) comprising at least one organic molecule according to the present invention.

[328] In the context of the present invention, the term "cyclic group" may be understood in the broadest sense as any mono-, bi- or polycyclic moiety.

[329] In the context of the present invention, the term "ring" when referring to chemical structures may be understood in the broadest sense as any monocyclic moiety. Along

the same lines, the term "rings" when referring to chemical structures may be understood in the broadest sense as any bi- or polycyclic moiety.

[330] In the context of the present invention, the term "ring system" may be understood in the broadest sense as any mono-, bi- or polycyclic moiety.

[331] In the context of the present invention, the term "ring atom" refers to any atom which is part of the cyclic core of a ring or a ring system, and not part of a non-cyclic substituent optionally attached to the cyclic core.

[332] In the context of the present invention, the term "carbocycle" may be understood in the broadest sense as any cyclic group in which the cyclic core structure comprises only carbon atoms that may of course be substituted with hydrogen or any other substituents defined in the specific embodiments of the invention. It is understood that the term "carbocyclic" as adjective refers to cyclic groups in which the cyclic core structure comprises only carbon atoms that may of course be substituted with hydrogen or any other substituents defined in the specific embodiments of the invention.

[333] In the context of the present invention, the term "heterocycle" may be understood in the broadest sense as any cyclic group in which the cyclic core structure comprises not just carbon atoms, but also at least one heteroatom. It is understood that the term "heterocyclic" as adjective refers to cyclic groups in which the cyclic core structure comprises not just carbon atoms, but also at least one heteroatom. The heteroatoms may, unless stated otherwise in specific embodiments, at each occurrence be the same or different and preferably be individually selected from the group consisting of B, Si, N, O, S, and Se, more preferably B, N, O and S, most preferably N, O, S. All carbon atoms or heteroatoms comprised in a heterocycle in the context of the invention may of course be substituted with hydrogen or any other substituents defined in the specific embodiments of the invention.

[334] The person skilled in the art understands that any cyclic group (i.e. any carbocycle and heterocycle) may be aliphatic or aromatic or heteroaromatic.

[335] In the context of the present invention, the term aliphatic when referring to a cyclic group (i.e. to a ring, to rings, to a ring system, to a carbocycle, to a heterocycle) means that the cyclic core structure (not counting substituents that are optionally attached to it) contains at least one ring atom that is not part of an aromatic or heteroaromatic ring or ring system. Preferably, the majority of ring atoms and more preferably all ring atoms within an aliphatic cyclic group are not part of an aromatic or heteroaromatic ring or ring system (such as in cyclohexane or in piperidine for example). Herein, no differentiation is made between carbocyclic and heterocyclic groups when referring to aliphatic rings or ring systems in general, whereas the term "aliphatic" may be used as adjective to describe a carbocycle or heterocycle in order to indicate whether or not a heteroatom is comprised in the aliphatic cyclic group.

[336] As understood by the skilled artisan, the terms "aryl" and "aromatic" may be understood in the broadest sense as any mono-, bi- or polycyclic aromatic moieties, i.e. cyclic groups in which all ring atoms are part of an aromatic ring system, preferably part of the same aromatic ring system. However, throughout the present application, the terms "aryl" and "aromatic" are restricted to mono-, bi- or polycyclic aromatic moieties wherein all aromatic ring atoms are carbon atoms. In contrast, the terms "heteroaryl" and "heteroaromatic" herein refer to any mono-, bi- or polycyclic aromatic moieties, wherein at least one aromatic carbon ring atom is replaced by a heteroatom (i.e. not carbon). Unless stated otherwise in specific embodiments of the invention, the at least one heteroatom within a "heteroaryl" or "heteroaromatic" may at each occurrence be the same or different and be individually selected from the group consisting of N, O, S, and Se, more preferably N, O, and S. The person skilled in the art understands that the adjectives "aromatic" and "heteroaromatic" may be used to describe any cyclic group (i.e. any ring system). This is to say that an aromatic cyclic group (i.e. an aromatic ring system) is an aryl group and a heteroaromatic cyclic group (i.e. a heteroaromatic ring system) is a heteroaryl group.

[337] Unless indicated differently in specific embodiments of the invention, an aryl group herein preferably contains 6 to 60 aromatic ring atoms, more preferably 6 to 40 aromatic ring atoms, and even more preferably 6 to 18 aromatic ring atoms. Unless indicated differently in specific embodiments of the invention, a heteroaryl group herein preferably contains 5 to 60 aromatic ring atoms, preferably 5 to 40 aromatic ring atoms, more preferably 5 to 20 aromatic ring atoms, out of which at least one is a heteroatom, preferably selected from N, O, S, and Se, more preferably from N, O, and S. If more than one heteroatom is comprised an a heteroaromatic group, all heteroatoms are preferably independently of each other selected from N, O, S, and Se, more preferably from N, O, and S.

[338] In the context of the present invention, for both aromatic and heteroaromatic groups (for example aryl or heteroaryl substituents), the number of aromatic ring carbon atoms may be given as subscripted number in the definition of certain substituents, for example in the form of "C_6-C_{60}-aryl", which means that the respective aryl substituent comprises 6 to 60 aromatic carbon ring atoms. The same subscripted numbers are herein also used to indicate the allowable number of carbon atoms in all other kinds of substituents, regardless of whether they are aliphatic, aromatic or heteroaromatic substituents. For example,

[339] the expression "C_1-C_{40}-alkyl" refers to an alkyl substituent comprising 1 to 40 carbon atoms.

[340] Preferred examples of aryl groups comprise groups derived from benzene, naphthalene, anthracene, phenanthrene, pyrene, dihydropyrene, chrysene, perylene,

fluoranthene, benzanthracene, benzophenanthrene, tetracene, pentacene, benzopyrene or combinations of these groups.

[341] Preferred examples of heteroaryl groups comprise groups derived from furan, benzofuran, isobenzofuran, dibenzofuran, thiophene, benzothiophene, isobenzothiophene, dibenzothiophene; pyrrole, indole, isoindole, carbazole, indolocarbazole, pyridine, quinoline, isoquinoline, acridine, phenanthridine, benzo-5,6-quinoline, benzo-6,7-quinoline, benzo-7,8-quinoline, phenothiazine, phenoxazine, pyrazole, indazole, imidazole, benzimidazole, naphthoimidazole, phenanthroimidazole, pyridoimidazole, pyrazinoimidazole, quinoxalinoimidazole, oxazole, benzoxazole, napthooxazole, anthroxazol, phenanthroxazol, isoxazole, 1,2-thiazole, 1,3-thiazole, benzothiazole, pyridazine, benzopyridazine, pyrimidine, benzopyrimidine, 1,3,5-triazine, 1,2,4-triazine, 1,2,3-triazine, quinoxaline, pyrazine, phenazine, naphthyridine, carboline, benzocarboline, phenanthroline, 1,2,3-triazole, 1,2,4-triazole, benzotriazole, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3,4-tetrazine, 1,2,4,5-tetrazine, purine, pteridine, indolizine and benzothiadiazole or combinations of these groups.

[342] As used throughout the present application, the term "arylene" refers to a divalent aryl substituent that bears two binding sites to other molecular structures, thereby serving as a linker structure. Along the same lines, the term "heteroarylene" refers to a divalent aryl substituent that bears two binding sites to other molecular structures, thereby serving as a linker structure.

[343] In the context of the present invention, the term "fused" when referring to aromatic or heteroaromatic ring systems means that the aromatic or hetroaromatic rings that are "fused" share at least one bond that is part of both ring systems. For example naphthalene (or naphthyl when referred to as substituent) or benzothiophene (or benzothiphenyl when referred to as substituent) are considered fused aromatic ring systems in the context of the present invention, in which two benzene rings (for naphthalene) or a thiophene and a benzene (for benzothiophene) share one bond. It is also understood that sharing a bond in this context includes sharing the two atoms that build up the respective bond and that fused aromatic or heteroaromatic ring systems can be understood as one aromatic or heteroaromatic ring system. Additionally, it is understood, that more than one bond may be shared by the aromatic or heteroaromatic rings building up a fused aromatic or heteroaromatic ring system (e.g. in pyrene). Furthermore, it will be understood that aliphatic ring systems may also be fused and that this has the same meaning as for aromatic or heteroaromatic ring systems, with the exception of course, that fused aliphatic ring systems are not aromatic. Furthermore, it is understood that an aromatic or heteroaromatic ring system may also be fused to (in other words: share at least one bond with) an aliphatic ring system.

[344] In the context of the present invention, the term "condensed" ring system has the same meaning as "fused" ring system.

[345] In certain embodiments of the invention, adjacent substituents bonded to a ring or a ring system may together form an additional mono- or polycyclic, aliphatic, aromatic or heteroaromatic ring system which is fused to the aromatic or heteroaromatic ring or ring system to which the substituents are bonded. It is understood that the optionally so formed fused ring system will be larger (meaning it comprises more ring atoms) than the aromatic or heteroaromatic ring or ring system to which the adjacent substituents are bonded. In these cases (and if such a number is provided), the "total" amount of ring atoms comprised in the fused ring system is to be understood as the sum of ring atoms comprised in the aromatic or heteroaromatic ring or ring system to which the adjacent substituents are bonded and the ring atoms of the additional ring system formed by the adjacent substituents, wherein, however, the ring atoms that are shared by fused rings are counted once and not twice. For example, a benzene ring may have two adjacent substituents that together form another benzene ring so that a naphthalene core is built. This naphthalene core then comprises 10 ring atoms as two carbon atoms are shared by the two benzene rings and are thus only counted once and not twice.

[346] In general, in the context of the present invention, the terms "adjacent substituents" or "adjacent groups" refer to substituents or groups bonded to either the same or to neighboring atoms.

[347] In the context of the present invention, the term "alkyl group" may be understood in the broadest sense as any linear, branched, or cyclic alkyl substituent. Preferred examples of alkyl groups as substituents comprise methyl (Me), ethyl (Et), n-propyl (^{n}Pr), i-propyl (^{i}Pr), cyclopropyl, n-butyl (^{n}Bu), i-butyl (^{i}Bu), s-butyl (^{s}Bu), t-butyl (^{t}Bu), cyclobutyl, 2-methylbutyl, n-pentyl, s-pentyl, t-pentyl, 2-pentyl, neo-pentyl, cyclopentyl, n-hexyl, s-hexyl, t-hexyl, 2-hexyl, 3-hexyl, neo-hexyl, cyclohexyl, 1-methylcyclopentyl, 2-methylpentyl, n-heptyl, 2-heptyl, 3-heptyl, 4-heptyl, cycloheptyl, 1-methylcyclohexyl, n-octyl, 2-ethylhexyl, cyclooctyl, 1-bicyclo[2,2,2]octyl, 2-bicyclo[2,2,2]-octyl, 2-(2,6-dimethyl)octyl, 3-(3,7-dimethyl)octyl, adamantyl1,1-dimethyl-n-hex-1-yl, 1,1-dimethyl-n-hept-1-yl, 1,1-dimethyl-n-oct-1-yl, 1,1-dimethyl-n-dec-1-yl, 1,1-dimethyl-n-dodec-1-yl, 1,1-dimethyl-n-tetradec-1-yl, 1,1-dimethyl-n-hexadec-1-yl, 1,1-dimethyl-n-octadec-1-yl, 1,1-diethyl-n-hex-1-yl, 1,1-diethyl-n-hept-1-yl, 1,1-diethyl-n-oct-1-yl, 1,1-diethyl-n-dec-1-yl, 1,1-diethyl-n-dodec-1-yl, 1,1-diethyl-n-tetradec-1-yl, 1,1-diethyln-n-hexadec-1-yl, 1,1-diethyl-n-octadec-1-yl, 1-(n-propyl)-cyclohex-1-yl, 1-(n-butyl)-cyclohex-1-yl, 1-(n-hexyl)-cyclohex-1-yl, 1-(n-octyl)-cyclohex-1-yl and 1-(n-decyl)-cyclohex-1-yl.

[348] The "s" in for example s-butyl, s-pentyl and s-hexyl refers to "secondary"; or in other words: s-butyl, s-pentyl and s-hexyl are equal to *sec*-butyl, *sec*-pentyl and *sec*-hexyl,

respectively. The "t" in for example t-butyl, t-pentyl and t-hexyl refers to "tertiary"; or in other words: t-butyl, t-pentyl and t-hexyl are equal to *tert*-butyl, *tert*-pentyl and *tert*-hexyl, respectively.

[349] As used herein, the term "alkenyl" comprises linear, branched, and cyclic alkenyl substituents. The term alkenyl group exemplarily comprises the substituents ethenyl, propenyl, butenyl, pentenyl, cyclopentenyl, hexenyl, cyclohexenyl, heptenyl, cycloheptenyl, octenyl, cyclooctenyl or cyclooctadienyl.

[350] As used herein, the term "alkynyl" comprises linear, branched, and cyclic alkynyl substituents. The term alkynyl group exemplarily comprises ethynyl, propynyl, butynyl, pentynyl, hexynyl, heptynyl or octynyl.

[351] As used herein, the term "alkoxy" comprises linear, branched, and cyclic alkoxy substituents. The term alkoxy group exemplarily comprises methoxy, ethoxy, n-propoxy, i-propoxy, n-butoxy, i-butoxy, s-butoxy, t-butoxy and 2-methylbutoxy.

[352] As used herein, the term "thioalkoxy" comprises linear, branched, and cyclic thioalkoxy substituents, in which the oxygen atom O of the corresponding alkoxy groups is replaced by sulfur, S.

[353] As used herein, the terms "halogen" (or "halo" when referred to as substituent in chemical nomenclature) may be understood in the broadest sense as any atom of an element of the 7th main group (in other words: group 17) of the periodic table of elements, preferably fluorine, chlorine, bromine or iodine.

[354] It is understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it was a fragment (e.g. naphthyl, dibenzofuryl) or as if it was the intact group (e.g. naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[355] Furthermore, herein, whenever a substituent such as "C_6-C_{60}-aryl" or "C_1-C_{40}-alkyl" is referred to without the name indicating the binding site within that substituent, this is to mean that the respective substituent may bond via any atom. For example, a "C_6-C_{60}-aryl"-substituent may bond via any of the 6 to 60 aromatic carbon atoms and a "C_1-C_{40}-alkyl"-substituent may bond via any of the 1 to 40 aliphatic carbon atoms. On the other hand, a "2-cyanophenyl"-substituent can only be bonded in such a way that its CN-group is adjacent to the binding site as to allow for the chemical nomenclature to be correct.

[356] In the context of the present invention, whenever a substituent such as "butyl", "biphenyl" or "terphenyl" is referred to without further detail, this is to mean that any isomer of the respective substituent is allowable as the specific substituent. In this regard, for example the term "butyl" as substituent comprises n-butyl, s-butyl, t-butyl, and iso-butyl as substituents. Along the same lines, the term "biphenyl" as substituent

comprises *ortho*-biphenyl, *meta*-biphenyl, or *para*-biphenyl, wherein ortho, meta and para are defined with regard to the binding site of the biphenyl substituent to the respective chemical moiety that bears the biphenyl substituent. Similarly, the term "terphenyl" as substituent comprises 3-*ortho*-terphenyl, 4-*ortho*-terphenyl, 4-*meta* -terphenyl, 5-*meta*-terphenyl, 2-*para*-terphenyl or 3-*para*-terphenyl, wherein, as known to the skilled artisan, *ortho*, *meta* and *para* indicate the position of the two Ph-moieties within the terphenyl-group to each other and "2-", "3-", "4-" and "5-" denotes the binding site of the terphenyl substituent to the respective chemical moiety that bears the terphenyl substituent.

[357] It is understood that all groups defined above and indeed all chemical moieties, regardless of whether they are cyclic or non-cyclic, aliphatic, aromatic or heteroaromatic, may be further substituted in accordance with the specific embodiments described herein.

[358] All hydrogen atoms (H) comprised in any structure referred to herein may at each occurrence independently and, be replaced by deuterium (D) without this being indicated specifically.The replacement of hydrogen by deuterium is common practice for the person skilled in the art. Thus, there are numerous known methods by which this can be achieved and several review articles describing them.

[359] If experimental or calculated data are compared, the values have to be determined by the same methodology. For example, if an experimental ΔE_{ST} is determined to be below 0.4 eV by a specific method, a comparison is only valid using the same specific method including the same conditions. To give a specific example, the comparison of the photoluminescence quantum yield (PLQY) of different compounds is only valid if the determination of the PLQY value was performed under the same reaction conditions (measurement in a 10% PMMA film at room temperature). Similarly, calculated energy values need to be determined by the same calculation method (using the same functional and the same basis set).

[360] <u>An optoelectronic device comprising at least one organic molecule according to the invention</u>

[361] A further aspect of the invention relates to an optoelectronic device comprising at least one organic molecule according to the present invention.

[362] In one embodiment, the optoelectronic device comprising at least one organic molecule according to the present invention is selected from the group consisting of:

[363] · organic light-emitting diodes (OLEDs),

[364] · light-emitting electrochemical cells,

[365] · OLED sensors, especially in gas and vapor sensors not hermetically externally shielded,

[366] · organic diodes,

[367] · organic solar cells,

[368] · organic transistors,

[369] · organic field-effect transistors,

[370] · organic lasers and

[371] · down-conversion elements.

[372] A light-emitting electrochemical cell consists of three layers, namely a cathode, an anode, and an active layer, which may contain the organic molecule according to the invention.

[373] In a preferred embodiment, the optoelectronic device comprising at least one organic molecule according to the present invention is selected from the group consisting of an organic light emitting diode (OLED), a light emitting electrochemical cell (LEC), an organic laser, and a light-emitting transistor.

[374] In an even more preferred embodiment, the optoelectronic device comprising at least one organic molecule according to the present invention is an organic light-emitting diode (OLED).

[375] The optoelectronic device of the invention may comprise a phosphorescence material comprising iridium in certain embodiments.

[376] In one embodiment, the optoelectronic device comprising at least one organic molecule according to the present invention is an OLED that may exhibit the following layer structure:

[377] 1. substrate

[378] 2. anode layer A

[379] 3. hole injection layer, HIL

[380] 4. hole transport layer, HTL

[381] 5. electron blocking layer, EBL

[382] 6. light-emitting layer (also referred to as emission layer), EML

[383] 7. hole blocking layer, HBL

[384] 8. electron transport layer, ETL

[385] 9. electron injection layer, EIL

[386] 10. cathode layer C,

[387] wherein the OLED comprises each layer, except for an anode layer A, a cathode layer C, and an EML, only optionally, and wherein different layers may be merged and the OLED may comprise more than one layer of each layer type defined above.

[388] Furthermore, the optoelectronic device comprising at least one organic molecule according to the present invention may optionally comprise one or more protective layers protecting the device from damaging exposure to harmful species in the environment including, exemplarily moisture, vapor and/or gases.

[389] In one embodiment, the optoelectronic device comprising at least one organic

molecule according to the present invention is an OLED, that may exhibit the following (inverted) layer structure:

[390] 1. substrate

[391] 2. cathode layer C

[392] 3. electron injection layer, EIL

[393] 4. electron transport layer, ETL

[394] 5. hole blocking layer, HBL

[395] 6. light-emitting layer (also referred to as emission layer), EML

[396] 7. electron blocking layer, EBL

[397] 8. hole transport layer, HTL

[398] 9. hole injection layer, HIL

[399] 10. anode layer A

[400] wherein the OLED (with an inverted layer structure) comprises each layer, except for an anode layer A, a cathode layer C, and an EML, only optionally, and wherein different layers may be merged and the OLED may comprise more than one layer of each layer types defined above.

[401] The organic molecules according to the invention (in accordance with the embodiments indicated above) can be employed in various layers, depending on the precise structure and on the substitution. In the case of the use, the fraction of the organic molecule according to the invention in the respective layer in an optoelectronic device, more particularly in an OLED, is 0.1% to 99% by weight, more particularly 1% to 80% by weight. In an alternative embodiment, the proportion of the organic molecule in the respective layer is 100% by weight.

[402] In one embodiment, of the optoelectronic device comprising at least one organic molecule according to the present invention is an OLED which may exhibit stacked architecture. In this architecture, contrary to the typical arrangement, where the OLEDs are placed side by side, the individual units are stacked on top of each other. Blended light may be generated with OLEDs exhibiting a stacked architecture, in particular white light may be generated by stacking blue, green and red OLEDs. Furthermore, the OLED exhibiting a stacked architecture may optionally comprise a charge generation layer (CGL), which is typically located between two OLED subunits and typically consists of a n-doped and p-doped layer with the n-doped layer of one CGL being typically located closer to the anode layer.

[403] In one embodiment, the optoelectronic device comprising at least one organic molecule according to the present invention is an OLED, which comprises two or more emission layers between anode and cathode. In particular, this so-called tandem OLED comprises three emission layers, wherein one emission layer emits red light, one emission layer emits green light and one emission layer emits blue light, and optionally

may comprise further layers such as charge generation layers, blocking or transporting layers between the individual emission layers. In a further embodiment, the emission layers are adjacently stacked. In a further embodiment, the tandem OLED comprises a charge generation layer between each two emission layers. In addition, adjacent emission layers or emission layers separated by a charge generation layer may be merged.

[404] In one embodiment, the optoelectronic device comprising at least one organic molecule according to the present invention may be an essentially white optoelectronic device, which is to say that the device emits white light. Exemplarily, such a white light-emitting optoelectronic device may comprise at least one (deep) blue emitter molecule and one or more emitter molecules emitting green and/or red light. Then, there may also optionally be energy transmittance between two or more molecules as described in a later section of this text (vide infra).

[405] In the case of the optoelectronic device comprising at least one organic molecule according to the present invention, it is preferred that the at least one organic molecule according to the present invention is comprised in a light-emitting layer (EML) of the optoelectronic device, most preferably in an EML of an OLED. However, the organic molecules according to the invention may for example also be employed in an electron transport layer (ETL) and/or in an electron blocking layer (EBL) or exciton-blocking layer and/or in a hole transport layer (HTL) and/or in a hole blocking layer (HBL). In the case of the use, the fraction of the organic molecule according to the invention in the respective layer in an optoelectronic device, more particularly in an OLED, is 0.1 % to 99 % by weight, more particularly 0.5 % to 80 % by weight, in particular 0.5 % to 10 % by weight. In an alternative embodiment, the proportion of the organic molecule in the respective layer is 100 % by weight.

[406] The selection criteria for suitable materials for the individual layers of optoelectronic devices, in particular OLEDs, are common knowledge of those skilled in the art. The state of the art describes plenty of materials to be used in the individual layers and also teaches which materials are suitable to be used alongside each other. It is understood that any materials used in the state of the art may also be used in optoelectronic devices comprising the organic molecule according to the present invention. In the following, preferred examples of materials for the individual layers will be given. It is understood that this does not imply that all types of layers listed below must be present in an opto-electronic device comprising at least one organic molecule according to the present invention. Additionally, it is understood that an optoelectronic device comprising at least one organic molecule according to the present invention may include more than one of each of the layers listed in the following, for example two or more light-emitting layers (EMLs). It is also understood that two or more layers of the same type

(e.g. two or more EMLs or two or more HTLs) do not necessarily comprise the same materials or even the same materials in the same ratios. Furthermore, it is understood that an optoelectronic device comprising at least one organic molecule according to the present invention does not have to comprise all the layer types listed in the following, wherein an anode layer, a cathode layer, and a light-emitting layer will usually be present in all cases.

[407] The substrate may be formed by any material or composition of materials. Most frequently, glass slides are used as substrates. Alternatively, thin metal layers (e.g., copper, gold, silver or aluminum films) or plastic films or slides may be used. This may allow a higher degree of flexibility. The anode layer A is mostly composed of materials allowing to obtain an (essentially) transparent film. As at least one of both electrodes should be (essentially) transparent in order to allow light emission from the OLED, either the anode layer A or the cathode layer C is usually transparent. Preferably, the anode layer A comprises a large content or even consists of transparent conductive oxides (TCOs). Such an anode layer A may, for example, comprise indium tin oxide, aluminum zinc oxide, fluorine doped tin oxide, indium zinc oxide, PbO, SnO, zirconium oxide, molybdenum oxide, vanadium oxide, wolfram oxide, graphite, doped Si, doped Ge, doped GaAs, doped polyaniline, doped polypyrrol and/or doped polythiophene.

[408] Preferably, an anode layer A (essentially) consists of indium tin oxide (ITO) (e.g., $(InO_3)_{0.9}(SnO_2)_{0.1}$). The roughness of an anode layer A caused by the transparent conductive oxides (TCOs) may be compensated by using a hole injection layer (HIL). Further, a HIL may facilitate the injection of quasi charge carriers (i.e., holes) in that the transport of the quasi charge carriers from the TCO to the hole transport layer (HTL) is facilitated. A hole injection layer (HIL) may comprise poly-3,4-ethylendioxy thiophene (PEDOT), polystyrene sulfonate (PSS), MoO_2, V_2O_5, CuPC or CuI, in particular a mixture of PEDOT and PSS. A hole injection layer (HIL) may also prevent the diffusion of metals from an anode layer A into a hole transport layer (HTL). A HIL may for example comprise PEDOT:PSS (poly-3,4-ethylendioxy thiophene: polystyrene sulfonate), PEDOT (poly-3,4-ethylendioxy thiophene), mMTDATA (4,4',4''-tris[phenyl(m-tolyl)amino]triphenylamine), Spiro-TAD (2,2',7,7'-tetrakis(n,n-diphenylamino)-9,9'-spirobifluorene), DNTPD (N1,N1'-(biphenyl-4,4'-diyl)bis(N1-phenyl-N4,N4-di-m-tolylbenzene-1,4-diamine), NPB (N,N'-bis-(1-naphthalenyl)-N,N'-bis-phenyl-(1,1'-biphenyl)-4,4'-diamine), NPNPB (N,N'-diphenyl-N,N'-di-[4-(N,N-diphenyl-amino)phenyl]benzidine), MeO-TPD (N,N,N',N''-tetrakis(4-methoxyphenyl)benzidine), HAT-CN (1,4,5,8,9,11-hexaazatriphenylen-hexacarbonitrile) and/or Spiro-NPD (N,N'-diphenyl-N,N'-bis-(1-naphthyl)-9,9'-spirobifluorene-2,7-diamine).

[409] Adjacent to an anode layer A or a hole injection layer (HIL), a hole transport layer (HTL) is typically located. Herein, any hole transport material may be used. Exemplarily, electron-rich heteroaromatic compounds such as triarylamines and/or carbazoles may be used as hole transport compound. A HTL may decrease the energy barrier between an anode layer A and a light-emitting layer EML. A hole transport layer (HTL) may also be an electron blocking layer (EBL). Preferably, hole transport compounds bear comparably high energy levels of their lowermost excited triplet states T1. Exemplarily, a hole transport layer (HTL) may comprise a star-shaped heterocyclic compound such as tris(4-carbazoyl-9-ylphenyl)amine (TCTA), poly-TPD (poly(4-butylphenyl-diphenyl-amine)), [alpha]-NPD (poly(4-butylphenyl-diphenyl-amine)), TAPC (4,4'-cyclohexyliden-bis[N,N-bis(4-methylphenyl)benzenamine]), 2-TNATA (4,4',4''-tris[2-naphthyl(phenyl)amino]triphenylamine), Spiro-TAD (2,2',7,7'-tetrakis(n,n-diphenylamino)-9,9'-spirobifluorene), DNTPD (N1,N1'-(biphenyl-4,4'-diyl)bis(N1-phenyl-N4,N4-di-m-tolylbenzene-1,4-diamine), NPB (N,N'-bis-(1-naphthalenyl)-N,N'-bis-phenyl-(1,1'-biphenyl)-4,4'-diamine)), NPNPB (N,N'-diphenyl-N,N'-di-[4-(N,N-diphenyl-amino)phenyl]benzidine), MeO-TPD (N,N,N',N'-tetrakis(4-methoxyphenyl)benzidine), HAT-CN (1,4,5,8,9,11-hexaazatriphenylen-hexacarbonitrile) and/or TrisPcz (9,9'-diphenyl-6-(9-phenyl-9H-carbazol-3-yl)-9H,9'H-3,3'-bicarbazole). In addition, a HTL may comprise a p-doped layer, which may be composed of an inorganic or organic dopant in an organic hole-transporting matrix. Transition metal oxides such as vanadium oxide, molybdenum oxide or tungsten oxide may be used as inorganic dopant. Tetrafluorotetracyanoquinodimethane (F4-TCNQ), copper-pentafluorobenzoate (Cu(I)pFBz) or transition metal complexes may be used as organic dopant.

[410] An EBL may for example comprise mCP (1,3-bis(carbazol-9-yl)benzene), TCTA (tris(4-carbazoyl-9-ylphenyl)amine), 2-TNATA (4,4',4''-tris[2-naphthyl(phenyl)amino]triphenylamine), mCBP (3,3-di(9H-carbazol-9-yl)biphenyl), tris-Pcz (9-Phenyl-3,6-bis(9-phenyl-9Hcarbazol-3-yl)-9H-carbazole), CzSi (9-(4-tert-Butylphenyl)-3,6-bis(triphenylsilyl)-9H-carbazole), and/or DCB (N,N'-dicarbazolyl-1,4-dimethylbenzene).

[411] Adjacent to a hole transport layer (HTL) or (if present) an electron blocking layer (EBL), typically, a light-emitting layer (EML) is located. A light-emitting layer (EML) comprises at least one light-emitting molecule (i.e. emitter material). Typically, an EML additionally comprises one or more host materials (also referred to as matrix materials). Exemplarily, the host material may be selected from CBP

(4,4'-Bis-(N-carbazolyl)-biphenyl), mCP (1,3-bis(carbazol-9-yl)benzene), mCBP (3,3-di(9H-carbazol-9-yl)biphenyl), Sif87 (dibenzo[b,d]thiophen-2-yltriphenylsilane), CzSi (9-(4-tert-Butylphenyl)-3,6-bis(triphenylsilyl)-9H-carbazole), Sif88 (dibenzo[b,d]thiophen-2-yl)diphenylsilane), DPEPO (bis[2-(diphenylphosphino)phenyl] ether oxide), 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzothiophen-2-yl)phenyl]-9H-carbazole, 9-[3,5-bis(2-dibenzofuranyl)phenyl]-9H-carbazole, 9-[3,5-bis(2-dibenzothiophenyl)phenyl]-9H-carbazole, T2T (2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine), T3T (2,4,6-tris(triphenyl-3-yl)-1,3,5-triazine) and/or TST (2,4,6-tris(9,9'-spirobifluorene-2-yl)-1,3,5-triazine). As known to the person skilled in the art, a host material typically should be selected to exhibit first (i.e. lowermost) excited triplet state (T1) and first (i.e. lowermost) excited singlet (S1) energy levels, which are energetically higher than the first (i.e. lowermost) excited triplet state (T1) and first (i.e. lowermost) excited singlet state (S1) energy levels of the at least one light-emitting molecule that is embedded in the respective host material(s).

[412] As stated previously, it is preferred that at least one EML of the optoelectronic device in the context of the invention comprises at least one molecule according to the present invention. The preferred compositions of an EML of an optoelectronic device comprising at least one organic molecule according to the present invention are described in more detail in a later section of this text (vide infra).

[413] Adjacent to a light-emitting layer (EML), an electron transport layer (ETL) may be located. Herein, any electron transport material may be used. Exemplarily, compounds bearing electron-deficient groups, such as for example benzimidazoles, pyridines, triazoles, triazines, oxadiazoles (e.g., 1,3,4-oxadiazole), phosphinoxides and sulfones, may be used. An electron transport material may also be a star-shaped heterocyclic compound such as 1,3,5-tri(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl (TPBi). An ETL may for example comprise NBphen (2,9-bis(naphthalen-2-yl)-4,7-diphenyl-1,10-phenanthroline), Alq3 (Aluminum-tris(8-hydroxyquinoline)), TSPO1 (diphenyl-4-triphenylsilylphenyl-phosphinoxide), BPyTP2 (2,7-di(2,2'-bipyridin-5-yl)triphenyle), Sif87 (dibenzo[b,d]thiophen-2-yltriphenylsilane), Sif88 (dibenzo[b,d]thiophen-2-yl)diphenylsilane), BmPyPhB (1,3-bis[3,5-di(pyridin-3-yl)phenyl]benzene) and/or BTB (4,4'-bis-[2-(4,6-diphenyl-1,3,5-triazinyl)]-1,1'-biphenyl). Optionally, an ETL may be doped with materials such as Liq ((8-hydroxyquinolinato)lithium). An electron

transport layer (ETL) may also block holes or a hole blocking layer (HBL) is introduced, typically between an EML and an ETL.

[414] A hole blocking layer (HBL) may for example comprise BCP (2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline = bathocuproine), 4,6-diphenyl-2-(3-(triphenylsilyl)phenyl)-1,3,5-triazine, 9,9'-(5-(6-([1,1'-biphenyl]-3-yl)-2-phenylpyrimidin-4-yl)-1,3-phenylene)bis(9H-carbazole), BAlq (bis(8-hydroxy-2-methylquinoline)-(4-phenylphenoxy)aluminum), NBphen (2,9-bis(naphthalen-2-yl)-4,7-diphenyl-1,10-phenanthroline), Alq3 (aluminum-tris(8-hydroxyquinoline)), TSPO1 (diphenyl-4-triphenylsilylphenyl-phosphinoxide), T2T (2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine), T3T (2,4,6-tris(triphenyl-3-yl)-1,3,5-triazine), TST (2,4,6-tris(9,9'-spirobifluorene-2-yl)-1,3,5-triazine), and/or TCB/TCP (1,3,5-tris(N-carbazolyl)benzol/ 1,3,5-tris(carbazol)-9-yl) benzene).

[415] A cathode layer C may be located adjacent to the electron transport layer (ETL). For example, the cathode layer C may comprise or may consist of a metal (e.g., Al, Au, Ag, Pt, Cu, Zn, Ni, Fe, Pb, LiF, Ca, Ba, Mg, In, W, or Pd) or a metal alloy. For practical reasons, the cathode layer may consist of (essentially) non-transparent metals such as Mg, Ca or Al. Alternatively or additionally, the cathode layer C may also comprise graphite and/or carbon nanotubes (CNTs). Alternatively, the cathode layer C may also comprise or consist of nanoscalic silver wires.

[416] An OLED comprising at least one organic molecule according to the present invention may further, optionally comprise a protection layer between an electron transport layer (ETL) and a cathode layer C (which may be designated as electron injection layer (EIL)). This layer may comprise lithium fluoride, cesium fluoride, silver, Liq ((8-hydroxyquinolinato)lithium), Li_2O, BaF_2, MgO and/or NaF.

[417] Optionally, an electron transport layer (ETL) and/or a hole blocking layer (HBL) may also comprise one or more host materials.

[418] As used herein, if not defined more specifically in the particular context, the designation of the colors of emitted and/or absorbed light is as follows:

[419] violet: wavelength range of >380-420 nm;

[420] deep blue: wavelength range of >420-480 nm;

[421] sky blue: wavelength range of >480-500 nm;

[422] green: wavelength range of >500-560 nm;

[423] yellow: wavelength range of >560-580 nm;

[424] orange: wavelength range of >580-620 nm;

[425] red: wavelength range of >620-800 nm.

[426] With respect to light-emitting molecules (in other words: emitter materials), such colors refer to the emission maximum of the main emission peak. Therefore, ex-

emplarily, a deep blue emitter has an emission maximum in the range of from >420 to 480 nm, a sky-blue emitter has an emission maximum in the range of from >480 to 500 nm, a green emitter has an emission maximum in a range of from >500 to 560 nm, and a red emitter has an emission maximum in a range of from >620 to 800 nm.

[427] A deep blue emitter may preferably have an emission maximum of below 475 nm, more preferably below 470 nm, even more preferably below 465 nm or even below 460 nm. It will typically be above 420 nm, preferably above 430 nm, more preferably above 440 nm or even above 450 nm. In a preferred embodiment, the organic molecules according to the present invention exhibit emission maxima between 420 and 500 nm, more preferably between 430 and 490 nm, even more preferably between 440 and 480 nm, and most preferably between 450 and 470 nm, typically measured at room temperature (i.e. (approximately) 20 °C) from a spin-coated film with 1-5 %, preferably 2 % by weight of the organic molecule according to the invention in poly(methyl methacrylate), PMMA, mCBP or alternatively in an organic solvent, preferably DCM or toluene, with 0.001 mg/mL of organic molecule according to the invention.

[428] A further embodiment relates to an OLED comprising at least one organic molecule according to the present invention and emitting light with CIEx and CIEy color co-ordinates close to the CIEx (= 0.131) and CIEy (= 0.046) color coordinates of the primary color blue (CIEx = 0.131 and CIEy = 0.046) as defined by the ITU-R Recommendation BT.2020 (Rec. 2020) and thus is suited for the use in Ultra High Definition (UHD) displays, e.g. UHD-TVs. Accordingly, a further aspect of the present invention relates to an OLED comprising at least one organic molecule according to the present invention, whose emission exhibits a CIEx color coordinate of between 0.02 and 0.30, preferably between 0.03 and 0.25, more preferably between 0.05 and 0.20 or even more preferably between 0.08 and 0.18 or even between 0.10 and 0.15 and/ or a CIEy color coordinate of between 0.00 and 0.45, preferably between 0.01 and 0.30, more preferably between 0.02 and 0.20 or even more preferably between 0.03 and 0.15 or even between 0.04 and 0.10.

[429] A further embodiment relates to an OLED comprising at least one organic molecule according to the present invention and exhibiting an external quantum efficiency at 1000 cd/m^2 of more than 8%, more preferably of more than 10%, more preferably of more than 13%, even more preferably of more than 15% or even more than 20% and/or exhibits an emission maximum 420 and 500 nm, more preferably between 430 and 490 nm, even more preferably between 440 and 480 nm, and most preferably between 450 and 470 nm or still and/or exhibits an LT80 value at 500 cd/m^2 of more than 100 h, preferably more than 200 h, more preferably more than 400 h, even more preferably more than 750 h or even more than 1000 h.

[430] A green emitter has an emission maximum of below 560 nm, more preferably below 550 nm, even more preferably below 545 nm or even below 540 nm. It will typically be above 500 nm, more preferably above 510 nm, even more preferably above 515 nm or even above 520 nm.

[431] A green emitter material may preferably have an emission maximum between 500 and 560 nm, more preferably between 510 and 550 nm, and even more preferably between 520 and 540 nm.

[432] In a further embodiment of the invention, the composition has a photoluminescence quantum yield (PLQY) of more than 20 %, preferably more than 30 %, more preferably more than 35 %, more preferably more than 40 %, more preferably more than 45 %, more preferably more than 50 %, more preferably more than 55 %, even more preferably more than 60 % or even more than 70 % at room temperature.

[433] A further preferred embodiment relates to an OLED comprising at least one organic molecule according to the present invention and emitting light at a distinct color point. Preferably, the OLED emits light with a narrow emission band (a small full width at half maximum (FWHM)). In a preferred embodiment, the OLED comprising at least one organic molecule according to the invention emits light with an FWHM of the main emission peak of less than 0.30 eV , preferably less than 25 eV, more preferably less than 0.20 eV, even more preferably less than 0.1 eV, or even less than 0.17 eV.

[434] In accordance with the invention, the optoelectronic devices comprising at least one organic molecule according to the present invention can for example be employed in displays, as light sources in lighting applications and as light sources in medical and/or cosmetic applications (for example light therapy).

[435] Combination of the organic molecules according to the invention with further materials

[436] It forms part of the common knowledge of those skilled in the art that any layer within an optoelectronic device (herein preferably an OLED), and in particular the light-emitting layer (EML), may be composed of a single material or a combination of different materials.

[437] For example, the person skilled in the art understands that an EML may be composed of a single material that is capable of emitting light when a voltage (and electrical current) is applied to said device. However, the skilled artisan also understands that it may be beneficial to combine different materials in an EML of an optoelectronic device (herein preferably an OLED), in particular one or more host material(s) (in other words: matrix material(s); herein designated host material(s) H^B when comprised in an optoelectronic device that comprises at least one organic molecule according to the invention) and one or more dopant materials out of which at least one is emissive (i.e. an emitter material) when applying a voltage and electrical current to the device.

[438] In a preferred embodiment of the use of an organic molecule according to the invention in an optoelectronic device, said optoelectronic device comprises at least one organic molecule according to the invention in an EML or in a layer that is directly adjacent to an EML or in more than one of these layers.

[439] In a preferred embodiment of the use of an organic molecule according to the invention in an optoelectronic device, said optoelectronic device is an OLED and comprises at least one organic molecule according to the invention in an EML or in a layer that is directly adjacent to an EML or in more than one of these layers.

[440] In an even more preferred embodiment of the use of an organic molecule according to the invention in an optoelectronic device, said optoelectronic device is an OLED and comprises at least one organic molecule according to the invention in an EML.

[441] In one embodiment relating to the optoelectronic device, preferably the OLED, comprising at least one organic molecule according to the invention, the at least one, preferably each, organic molecule according to the invention is used as emitter material in a light-emitting layer EML, which is to say that it emits light when a voltage (and electrical current) is applied to said device.

[442] As known to the person skilled in the art, light emission from emitter materials (i.e. emissive dopants), for example in organic light-emitting diodes (OLEDs), may comprise fluorescence from excited singlet states (typically the lowermost excited singlet state S1) and phosphorescence from excited triplet states (typically the lowermost excited triplet state T1).

[443] A fluorescence emitter F is capable of emitting light at room temperature (i.e. (approximately) 20 °C) upon electronic excitation (for example in an optoelectronic device), wherein the emissive excited state is a singlet state. Fluorescence emitters usually display prompt (i.e. direct) fluorescence on a timescale of nanoseconds, when the initial electronic excitation (for example by electron hole recombination) affords an excited singlet state of the emitter.

[444] In the context of the invention, a delayed fluorescence material is a material that is capable of reaching an excited singlet state (typically the lowermost excited singlet state S1) by means of reverse intersystem crossing (RISC; in other words: up intersystem crossing or inverse intersystem crossing) from an excited triplet state (typically from the lowermost excited triplet state T1) and that is furthermore capable of emitting light when returning from the so-reached excited singlet state (typically S1) to its electronic ground state. The fluorescence emission observed after RISC from an excited triplet state (typically T1) to the emissive excited singlet state (typically S1) occurs on a timescale (typically in the range of microseconds) that is slower than the timescale on which direct (i.e. prompt) fluorescence occurs (typically in the range of nanoseconds) and is thus referred to as delayed fluorescence (DF). When RISC from

an excited triplet state (typically from T1) to an excited singlet state (typically to S1), occurs through thermal activation, and if the so populated excited singlet state emits light (delayed fluorescence emission), the process is referred to as thermally activated delayed fluorescence (TADF). Accordingly, a TADF material is a material that is capable of emitting thermally activated delayed fluorescence (TADF) as explained above. It is known to the person skilled in the art that, when the energy difference ΔE_{ST} between the lowermost excited singlet state energy level $E(S1^E)$ and the lowermost excited triplet state energy level $E(T1^E)$ of a fluorescence emitter F is reduced, population of the lowermost excited singlet state from the lowermost excited triplet state by means of RISC may occur with high efficiency. Thus, it forms part of the common knowledge of those skilled in the art that a TADF material will typically have a small ΔE_{ST} value (vide infra). As known to the person skilled in the art, a TADF material may not just be a material that is on its own capable of RISC from an excited triplet state to an excited singlet state with subsequent emission of TADF as laid out above. It is known to those skilled in the art that a TADF material may in fact also be an exciplex that is formed from two kinds of materials, preferably from two host materials H^B, more preferably from a p-host material H^P and an n-host material H^N (vide infra).

[445] The occurrence of (thermally activated) delayed fluorescence may for example be analyzed based on the decay curve obtained from time-resolved (i.e. transient) photoluminescence (PL) measurements. For this purpose, a spin-coated film of the respective emitter (i.e. the assumed TADF material) in poly(methyl methacrylate) (PMMA) with 1-10% by weight, in particular 10% by weight of the respective emitter may be used as sample. The analysis may for example be performed using an FS5 fluorescence spectrometer from Edinburgh instruments. The sample PMMA film may be placed in a cuvette and kept under nitrogen atmosphere during the measurement. Data acquisition may be performed using the well-established technique of time correlated single photon counting (TCSPC, vide infra). To gather the full decay dynamics over several orders of magnitude in time and signal intensity, measurements in four time windows (200 ns, 1 μs, and 20 μs, and a longer measurement spanning > 80 μs) may be carried out and combined (vide infra).

[446] TADF materials preferably fulfill the following two conditions regarding the aforementioned full decay dynamics:

[447] (i) the decay dynamics exhibit two time regimes, one in the nanosecond (ns) range and the other in the microsecond (μs) range; and

[448] (ii) the shapes of the emission spectra in both time regimes coincide;

[449] wherein, the fraction of light emitted in the first decay regime is taken as prompt fluorescence and the fraction emitted in the second decay regime is taken as delayed fluo-

rescence.

[450] The ratio of delayed and prompt fluorescence may be expressed in form of a so-called n-value that may be calculated by the integration of respective photoluminescence decays in time according to the following equation:

[451] $$\frac{\int I_{DF}(t)dt}{\int I_{PF}(t)dt} = n$$

[452] In the context of the present invention, a TADF material preferably exhibits an n-value (ratio of delayed to prompt fluorescence) larger than 0.05 (n > 0.05), more preferably larger than 0.1 (n > 0.1), even more preferably larger than 0.15 (n > 0.15), particularly preferably larger than 0.2 (n > 0.20), or even larger than 0.25 (n > 0.25).

[453] In a preferred embodiment, the organic molecules according to the invention exhibit an n-value (ratio of delayed to prompt fluorescence) larger than 0.05 (n > 0.05).

[454] In the context of the present invention, a TADF material E^B is characterized by exhibiting a ΔE_{ST} value, which corresponds to the energy difference between the lowermost excited singlet state energy level $E(S1^E)$ and the lowermost excited triplet state energy level $E(T1^E)$, of less than 0.4 eV, preferably of less than 0.3 eV, more preferably of less than 0.2 eV, even more preferably of less than 0.1 eV, or even of less than 0.05 eV. The means of determining the ΔE_{ST} value of TADF materials E^B are laid out in a later subchapter of this text.

[455] One approach for the design of TADF materials in general is to covalently attach one or more (electron) donor moieties on which the HOMO is distributed and one or more (electron) acceptor moieties on which the LUMO is distributed to the same bridge, herein referred to as linker group. A TADF material E^B may, for example, also comprise two or three linker groups which are bonded to the same acceptor moiety and additional donor and acceptor moieties may be bonded to each of these two or three linker groups.

[456] One or more donor moieties and one or more acceptor moieties may also be bonded directly to each other (without the presence of a linker group).

[457] Typical donor moieties are derivatives of diphenyl amine, indole, carbazole, acridine, phenoxazine, and related structures. In particular, aliphatic, aromatic or heteroaromatic ring systems may be fused to the aforementioned donor motifs to arrive at for example indolocarbazoles.

[458] Benzene-, biphenyl-, and to some extend also terphenyl-derivatives are common linker groups.

[459] Nitrile groups are common acceptor moieties in TADF materials and known examples thereof include:

[460] (i) carbazolyl dicyanobenzene compounds

[461] such as 2CzPN (4,5-di(9*H*-carbazol-9-yl)phthalonitrile), DCzIPN (4,6-di(9*H*-carbazol-9-yl)isophthalonitrile), 4CzPN (3,4,5,6-tetra(9*H*-carbazol-9-yl)phthalonitrile), 4CzIPN (2,4,5,6-Tetra(9*H*-carbazol-9-yl)isophthalonitrile), 4CzTPN (2,4,5,6-tetra(9*H*-carbazol-9-yl)terephthalonitrile), and derivatives thereof;

[462] (ii) carbazolyl cyanopyridine compounds

[463] such as 4CzCNPy (2,3,5,6-tetra(9*H*-carbazol-9-yl)-4-cyanopyridine) and derivatives thereof;

[464] (iii) carbazolyl cyanobiphenyl compounds

[465] such as CNBPCz (4,4',5,5'-tetra(9*H*-carbazol-9-yl)-[1,1'-biphenyl]-2,2'-dicarbonitrile), CzBPCN (4,4',6,6'-tetra(9*H*-carbazol-9-yl)-[1,1'-biphenyl]-3,3'-dicarbonitrile), DDCzIPN (3,3',5,5'-tetra(9*H*-carbazol-9-yl)-[1,1'-biphenyl]-2,2',6,6'-tetracarbonitrile) and derivatives thereof;

[466] wherein in these materials, one or more of the nitrile groups may be replaced my fluorine (F) or trifluoromethyl (CF_3) as acceptor moieties.

[467] Nitrogen-heterocycles such as triazine-, pyrimidine-, triazole-, oxadiazole-, thiadiazole-, heptazine-, 1,4-diazatriphenylene-, benzothiazole-, benzoxazole-, quinoxaline-, and diazafluorene-derivatives are also well-known acceptor moieties used for the construction of TADF molecules. Known examples of TADF molecules comprising for example a triazine acceptor include PIC-TRZ (7,7'-(6-([1,1'-biphenyl]-4-yl)-1,3,5-triazine-2,4-diyl)bis(5-phenyl-5,7-dihydroindolo[2,3-b]carbazole)), *m*BFCzTrz (5-(3-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-5*H*-benzofuro[3,2-c]carbazole), and DCzTrz (9,9'-(5-(4,6-diphenyl-1,3,5-triazin-2-yl)-1,3-phenylene)bis(9H-carbazole)).

[468] Another group of TADF materials comprises diaryl ketones such as benzophenone or (heteroaryl)aryl ketones such as 4-benzoylpyridine, 9,10-anthraquinone, 9*H*-xanthen-9-one, and derivatives thereof as acceptor moieties to which the donor moieties (usually carbazolyl substituents) are bonded. Examples of such TADF molecules include BPBCz (bis(4-(9'-phenyl-9*H*,9'*H*-[3,3'-bicarbazol]-9-yl)phenyl)methanone), mDCBP ((3,5-di(9*H*-carbazol-9-yl)phenyl)(pyridin-4-yl)methanone), AQ-DTBu-Cz (2,6-bis(4-(3,6-di-*tert*-butyl-9*H*-carbazol-9-yl)phenyl)anthracene-9,10-dione), and MCz-XT (3-(1,3,6,8-tetramethyl-9*H*-carbazol-9-yl)-9*H*-xanthen-9-one), respectively.

[469] Sulfoxides, in particular diphenyl sulfoxides, are also commonly used as acceptor moieties for the construction of TADF materials and known examples include 4-PC-DPS (9-phenyl-3-(4-(phenylsulfonyl)phenyl)-9*H*-carbazole), DitBu-DPS (9,9'-(sulfonylbis(4,1-phenylene))bis(9*H*-carbazole)), and TXO-PhCz (2-(9-phenyl-9*H*-carbazol-3-yl)-9*H*-thioxanthen-9-one 10,10-dioxide).

[470] It is understood that a fluorescence emitter F may also display TADF as defined

herein and even be a TADF material E^B as defined herein. In consequence, a small FWHM emitter S^B as defined herein may or may not also be a TADF material E^B as defined herein.

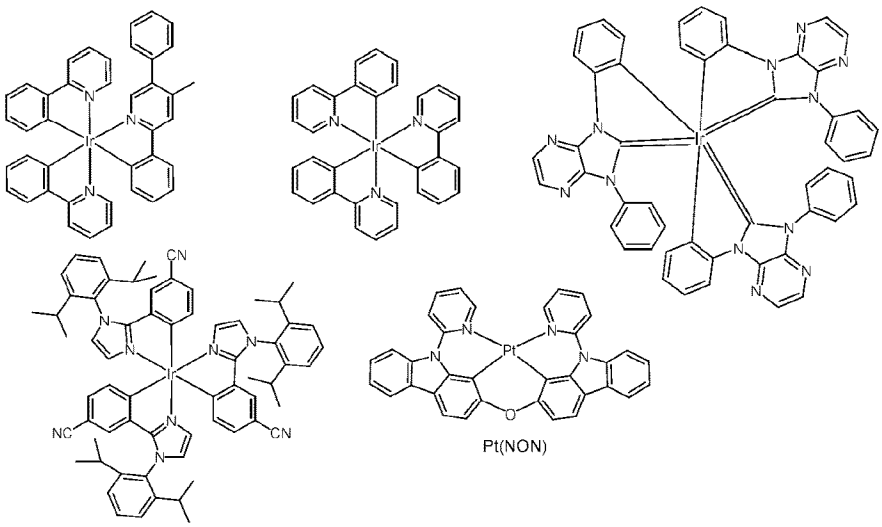
[471] Phosphorescence, i.e. light emission from excited triplet states (typically from the lowermost excited triplet state T1) is a spin-forbidden process. As known to the person skilled in the art, phosphorescence may be facilitated (enhanced) by exploiting the (intramolecular) spin-orbit interaction (so called (internal) heavy atom effect). A phosphorescence material P^B in the context of the invention is a phosphorescence emitter capable of emitting phosphorescence at room temperature (i.e. at approximately 20 °C).

[472] Herein, it is preferred that a phosphorescence material P^B comprises at least one atom of an element having a standard atomic weight larger than the standard atomic weight of calcium (Ca). Even more preferably, a phosphorescence material P^B in the context of the invention comprises a transition metal atom, in particular a transition metal atom of an element having a standard atomic weight larger than the standard atomic weight of zinc (Zn). The transition metal atom preferably comprised in the phosphorescence material P^B may be present in any oxidation state (and may also be present as ion of the respective element).

[473] It is common knowledge to those skilled in the art that phosphorescence materials P^B used in optoelectronic devices are oftentimes complexes of Ir, Pd, Pt, Au, Os, Eu, Ru, Re, Ag and Cu, in the context of this invention preferably of Ir, Pt, and Pd, more preferably of Ir and Pt. The skilled artisan knows which materials are suitable as phosphorescence materials P^B in optoelectronic devices and how to synthesize them. Furthermore, the skilled artisan is familiar with the design principles of phosphorescent complexes for use as phosphorescence materials in optoelectronic devices and knows how to tune the emission of the complexes by means of structural variations.

[474] The skilled artisan knows which materials are suitable as phosphorescence materials P^B to be used in optoelectronic devices and how to synthesize them. In this regard, the skilled artisan is in particular familiar with the design principles of phosphorescent complexes for use as phosphorescence materials P^B in optoelectronic devices and knows how to tune the emission of the complexes by means of structural variations.

[475] Examples of phosphorescence materials P^B that may be used alongside the organic molecules according to the present invention (for example in form of a composition or in an EML of an optoelectronic device, vide infra) are disclosed in the state of the art. For example, the following metal complexes are phosphorescence materials P^B that may be used alongside the organic molecules according to the present invention:

[476] 

[477] A small full width at half maximum (FWHM) emitter S^B in the context of the invention is any emitter (i.e. emitter material) that has an emission spectrum, which exhibits an FWHM of less than or equal to 0.35 eV (≤0.35 eV), preferably of less than or equal to 0.30 eV (≤0.30 eV), in particular of less than or equal to 0.25 eV (≤0.25 eV). Unless stated otherwise, this is judged based on an emission spectrum of the respective emitter at room temperature (i.e., (approximately) 20 °C), typically measured with 1 to 5% by weight, in particular with 2% by weight, of the emitter in poly(methyl methacrylate) PMMA or mCBP. Alternatively, emission spectra of small FWHM emitters S^B may be measured in a solution, typically with 0.001-0.2 mg/mL of the emitter S^B in dichloromethane or toluene at room temperature (i.e., (approximately) 20 °C).

[478] A small FWHM emitter S^B may be a fluorescence emitter F, a phosphorescence emitter (for example a phosphorescence material P^B) and/or a TADF emitter (for example a TADF material E^B). For TADF materials E^B and for phosphorescence materials P^B as laid out above, the emission spectrum is recorded at room temperature (i.e. approximately 20°C) from a spin-coated film of the respective material in poly(methyl methacrylate) PMMA, with 10% by weight of the respective molecule of the invention, E^B or P^B.

[479] As known to the person skilled in the art, the full width at half maximum (FWHM) of an emitter (for example a small FWHM emitter S^B) is readily determined from the respective emission spectrum (fluorescence spectrum for fluorescence emitters and phosphorescence spectrum for phosphorescence emitters). All reported FWHM values typically refer to the main emission peak (i.e. the peak with the highest intensity). The means of determining the FWHM (herein preferably reported in electron volts, eV) are part of the common knowledge of those skilled in the art. Given for example that the main emission peak of an emission spectrum reaches its half maximum emission (i.e.

50% of the maximum emission intensity) at the two wavelengths λ_1 and λ_2, both obtained in nanometers (nm) from the emission spectrum, the FWHM in electron volts (eV) is commonly (and herein) determined using the following equation:

[480] $$\text{FWHM [eV]} = \left| \frac{1239.84\,[eV \cdot nm]}{\lambda_2\,[nm]} - \frac{1239.84[eV \cdot nm]}{\lambda_1\,[nm]} \right|$$

[481] In the context of the invention, a small FWHM emitter S^B is an organic emitter, which, in the context of the invention, means that it does not contain any transition metals. Preferably, a small FWHM emitter S^B in the context of the invention predominantly consists of the elements hydrogen (H), carbon (C), nitrogen (N), and boron (B), but may for example also comprise oxygen (O), silicon (Si), fluorine (F), and bromine (Br).

[482] Furthermore, it is preferred that a small FWHM emitter S^B in the context of the invention is a fluorescence emitter F that may or may not additionally exhibit TADF.

[483] Preferably, a small FWHM emitter S^B in the context of the invention preferably fulfills at least one of the following requirements:

[484] (i) it is a boron (B)-containing emitter, which means that at least one atom within the respective small FWHM emitter S^B is boron (B);

[485] (ii) it comprises a polycyclic aromatic or heteroaromatic core structure, wherein at least two aromatic rings are fused together (e.g. anthracene, pyrene or aza-derivatives thereof).

[486] As known to person skilled in the art, a host material H^B of an EML may transport electrons or positive charges through said EML and may also transfer excitation energy to the at least one emitter material doped in the host material(s) H^B. The skilled artisan understands that a host material H^B comprised in an EML of an optoelectronic device (e.g. an OLED) is typically not significantly involved in light emission from said device upon applying a voltage and electrical current. The person skilled in the art is also familiar with the fact that any host material H^B may be a p-host H^P exhibiting high hole mobility, an n-host H^N exhibiting high electron mobility, or a bipolar host material H^{BP} exhibiting both, high hole mobility and high electron mobility.

[487] As known to person skilled in the art, an EML may also comprise a so-called mixed-host system with at least one p-host H^P and one n-host H^N. In particular, the EML may comprise exactly one emitter material according to the invention and a mixed-host system comprising T2T (2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine) as n-host H^N and a host selected from CBP, mCP, mCBP,
4,6-diphenyl-2-(3-(triphenylsilyl)phenyl)-1,3,5-triazine,
9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole,
9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole,
9-[3-(dibenzothiophen-2-yl)phenyl]-9H-carbazole,

9-[3,5-bis(2-dibenzofuranyl)phenyl]-9H-carbazole and

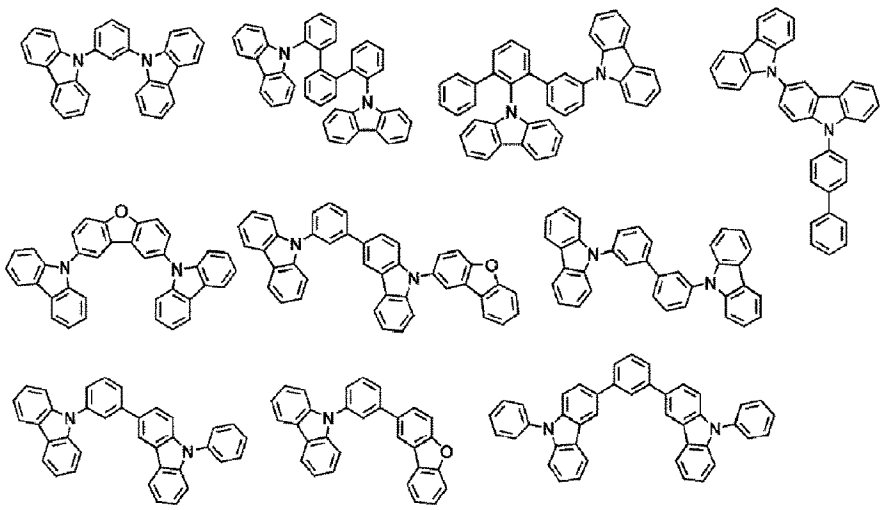
9-[3,5-bis(2-dibenzothiophenyl)phenyl]-9H-carbazole as p-host H^P.

[488] An EML may comprise a so-called mixed-host system with at least one p-host H^P and one n-host H^N; wherein the n-host H^N comprises groups derived from pyridine, pyrimidine, benzopyrimidine, 1,3,5-triazine, 1,2,4-triazine, and 1,2,3-triazine, while the p-host H^P comprises groups derived from indole, isoindole, and preferably carbazole.

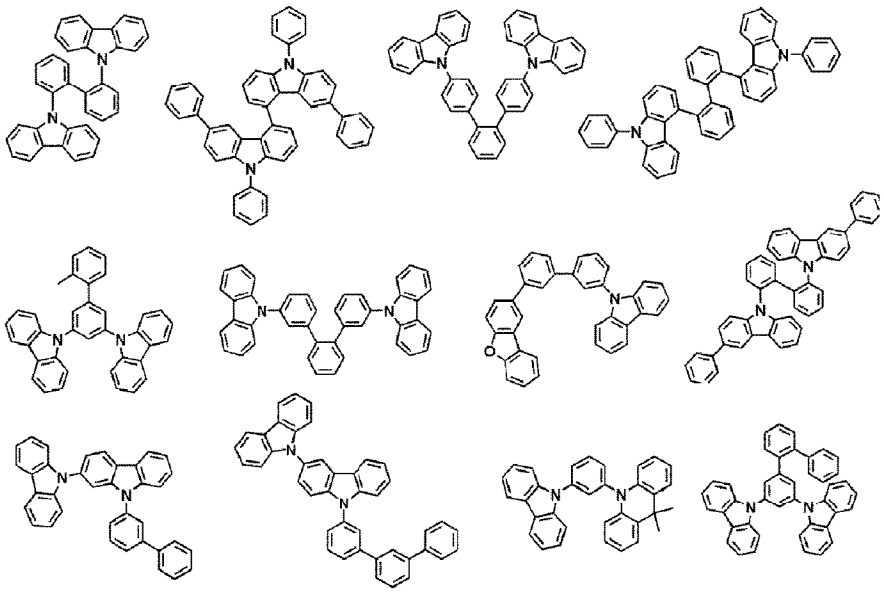
[489] The person skilled in the art knows which materials are suitable host materials for use in optoelectronic devices. It is understood that any host materials that are used in the state of the art may be suitable host materials H^B in the context of the invention.

[490] Examples of materials H^B that are p-host materials H^P in the context of the invention are listed below:

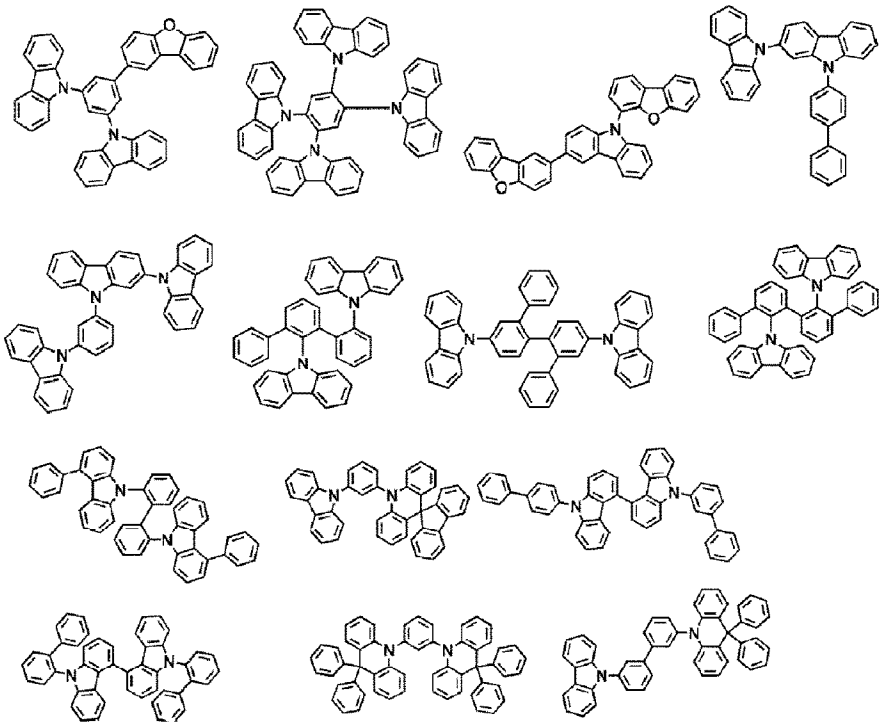
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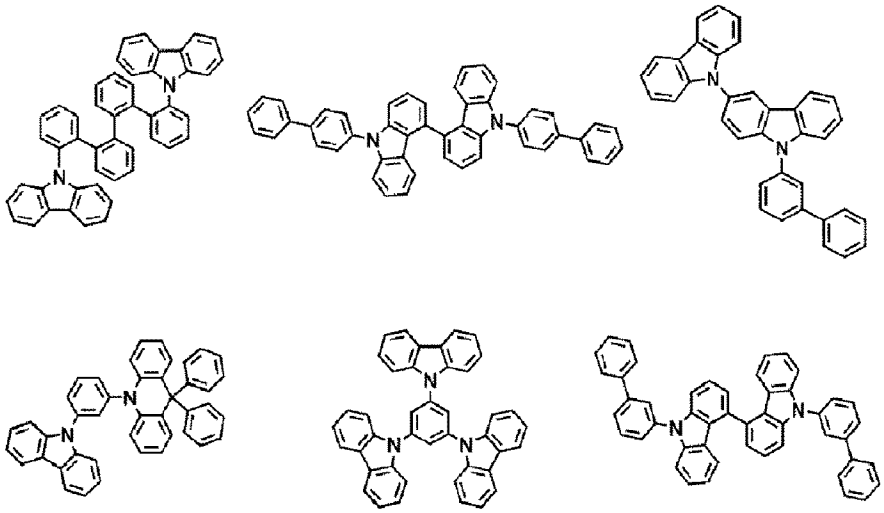
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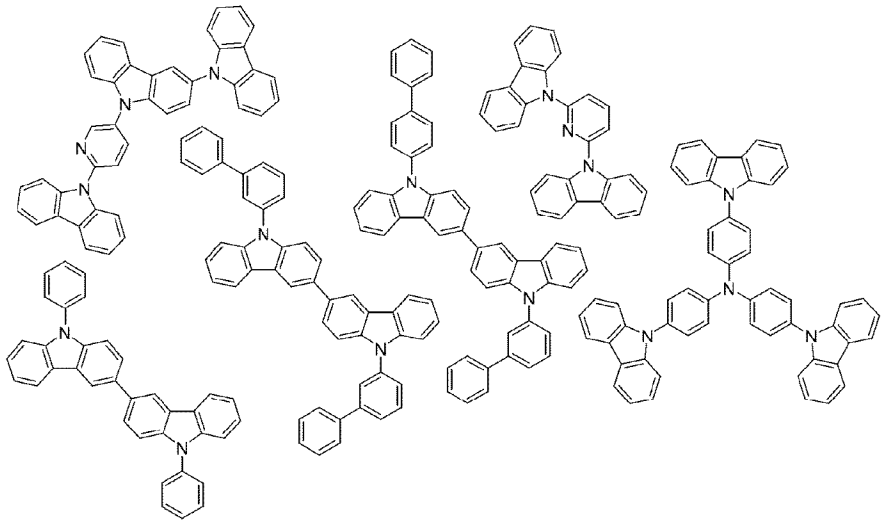
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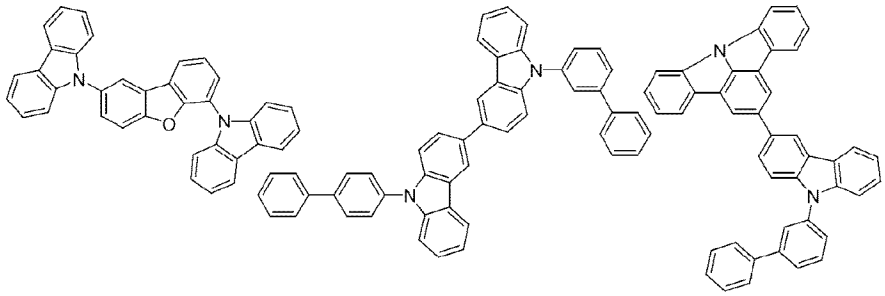


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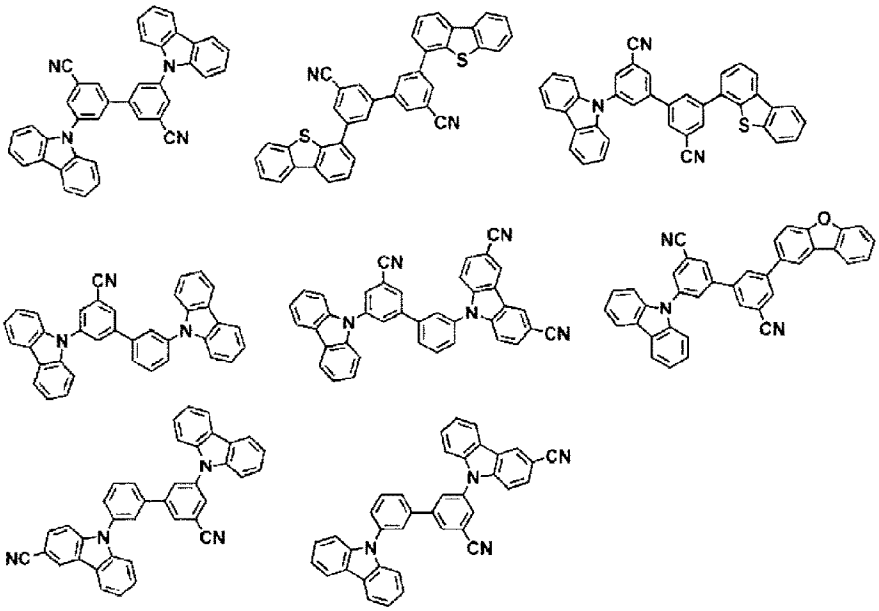


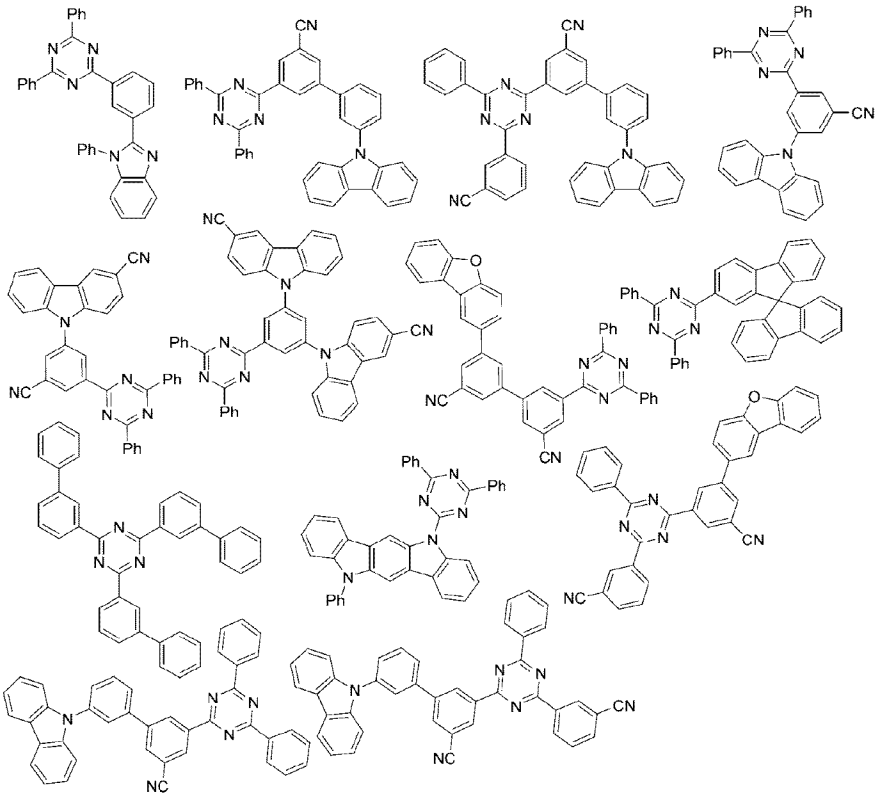
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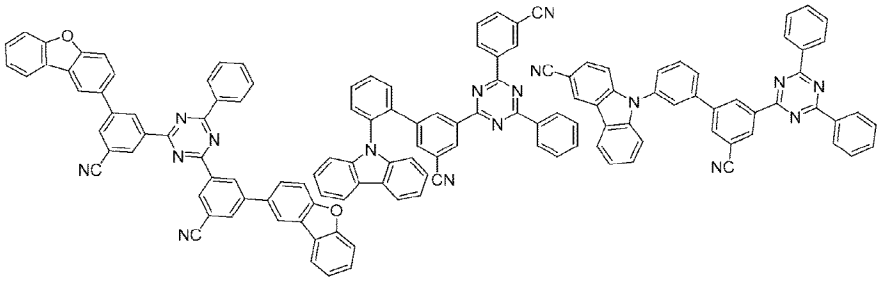


[496] 

[497] Examples of materials H^B that are n-host materials H^N in the context of the invention are listed below:

[498] 

[499] 

[500] 

[501] The person skilled in the art understands that any materials that are comprised in the same layer, in particular in the same EML, but also materials that are in adjacent layers and get in close proximity at the interface between these adjacent layers, may together form an exciplex. The person skilled in the art knows how to choose pairs of materials, in particular pairs of a p-host H^P and an n-host H^N, which form an exciplex and the selection criteria for the two components of said pair of materials, including HOMO- and/or LUMO-energy level requirements. This is to say that, in case exciplex formation may be aspired, the highest occupied molecular orbital (HOMO) of the one component, e.g. the p-host material H^P, may be at least 0.20 eV higher in energy than the HOMO of the other component, e.g. the n-host material H^N, and the lowest un-occupied molecular orbital (LUMO) of the one component, e.g. the p-host material H^P, may be at least 0.20 eV higher in energy than the LUMO of the other component, e.g. the n-host material H^N. It belongs to the common knowledge of those skilled in the art that, if present in an EML of an optoelectronic device, in particular an OLED, an

exciplex may have the function of an emitter material and emit light when a voltage and electrical current are applied to said device. As also commonly known from the state of the art, an exciplex may also be non-emissive and may for example transfer excitation energy to an emitter material, if comprised in an EML of an optoelectronic device.

[502] As known to a person skilled in the art, triplet-triplet annihilation (TTA) materials can be used as host materials H^B. The TTA material enables triplet-triplet annihilation. Triplet-triplet annihilation may preferably result in a photon up-conversion. Accordingly, two, three or even more photons may facilitate photon up-conversion from the lowermost excited triplet state ($T1^{TTA}$) to the first excited singlet state $S1^{TTA}$ of the TTA material H^{TTA}. In a preferred embodiment, two photons facilitate photon up-conversion from $T1^{TTA}$ to $S1^{TTA}$. Triplet-triplet annihilation may thus be a process that through a number of energy transfer steps, may combine two (or optionally more than two) low frequency photons into one photon of higher frequency.

[503] Optionally, the TTA material may comprise an absorbing moiety, the sensitizer moiety, and an emitting moiety (or annihilator moiety). In this context, an emitter moiety may, for example, be a polycyclic aromatic moiety such as, benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene. In a preferred embodiment, the polycyclic aromatic moiety comprises an anthracene moiety or a derivative thereof. A sensitizer moiety and an emitting moiety may be located in two different chemical compounds (i.e., separated chemical entities) or may be both moieties embraced by one chemical compound.

[504] According to the invention, a triplet-triplet annihilation (TTA) material converts energy from first excited triplet states $T1^N$ to first excited singlet states $S1^N$ by triplet-triplet annihilation.

[505] According to the present invention, a TTA material is characterized in that it exhibits triplet-triplet annihilation from the lowermost excited triplet state ($T1^N$) resulting in a triplet-triplet annihilated first excited singlet state $S1^N$, having an energy of up to two times the energy of $T1^N$.

[506] In one embodiment of the present invention, a TTA material is characterized in that it exhibits triplet-triplet annihilation from $T1^N$ resulting in $S1^N$, having an energy of 1.01 to 2fold, 1.1 to 1.9fold, 1.2 to 1.5fold, 1.4 to 1.6fold, or 1.5 to 2fold times the energy of $T1^N$.

[507] As used herein, the terms "TTA material" and "TTA compound" may be understood interchangeably.

[508] Typical "TTA material" can be found in the state of the art related to blue fluorescent OLEDs, as described by Kondakov (Philosophical Transactions of the Royal Society

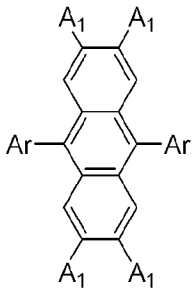
A: Mathematical, Physical and Engineering Sciences, 2015, 373:20140321). Such blue fluorescent OLEDs employ aromatic hydrocarbons such as anthracene derivatives as the main component (host) in the EML.

[509] In a preferred embodiment, the TTA material enables sensitized triplet-triplet annihilation. Optionally, the TTA material may comprise one or more polycyclic aromatic structures. In a preferred embodiment, the TTA material comprises at least one polycyclic aromatic structure and at least one further aromatic residue.

[510] In a preferred embodiment, the TTA material bears larger singlet-triplet energy splitting, i.e., an energy difference between its first excited singlet state $S1^N$ and its lowermost excited triplet state $T1^N$ of at least 1.1fold, at least 1.2fold, at least 1.3fold, at least 1.5fold and preferably not more than 2fold.

[511] In a preferred embodiment of the invention, the TTA material H^{TTA} is an anthracene derivative.

[512] In one embodiment, the TTA material H^{TTA} is an anthracene derivate of the following formula 4

[513] 

[514] Formula 4,

[515] wherein

[516] each Ar is independently from each other selected from the group consisting of C_6-C_{60}-aryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40}-(hetero)alkyl;

[517] and C_3-C_{57}-heteroaryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40}-(hetero)alkyl; and

[518] each A_1 is independently from each other selected from the group consisting of consisting of

[519] hydrogen;

[520] deuterium;

[521] C_6-C_{60}-aryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40} -(hetero)alkyl; C_3-C_{57}-heteroaryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen,

and C_1-C_{40}-(hetero)alkyl; and

[522] C_1-C_{40}-(hetero)alkyl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40}-(hetero)alkyl.

[523] In one embodiment, the TTA material H^{TTA} is an anthracene derivate of the following formula 4, wherein

[524] each Ar is independently from each other selected from the group consisting of C_6-C_{20}-aryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{20}-aryl, C_3-C_{20}-heteroaryl, halogen, and C_1-C_{210}-(hetero)alkyl;

[525] and C_3-C_{20}-heteroaryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{20}-aryl, C_3-C_{20}-heteroaryl, halogen, and C_1-C_{10}-(hetero)alkyl; and

[526] each A_1 is independently from each other selected from the group consisting of consisting of

[527] hydrogen,

[528] deuterium,

[529] C_6-C_{20}-aryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{20}-aryl, C_3-C_{20}-heteroaryl, halogen, and C_1-C_{10} -(hetero)alkyl,

[530] C_3-C_{20}-heteroaryl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{20}-aryl, C_3-C_{20}-heteroaryl, halogen, and C_1-C_{10} -(hetero)alkyl; and

[531] C_1-C_{10}-(hetero)alkyl, which is optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40}-(hetero)alkyl.

[532] In one embodiment, H^{TTA} is an anthracene derivate of the following formula 4, wherein at least one of A_1 is hydrogen. In one embodiment, H^{TTA} is an anthracene derivate of the following formula 4, wherein at least two of A_1 are hydrogen. In one embodiment, H^{TTA} is an anthracene derivate of the following formula 4, wherein at least three of A_1 are hydrogen. In one embodiment, H^{TTA} is an anthracene derivate of the following formula 4, wherein all of A_1 are each hydrogen.

[533] In one embodiment, H^{TTA} is an anthracene derivate of the following formula 4, wherein one of Ar is a residue selected from the group consisting of phenyl, naphthyl, phenanthryl, pyrenyl, triphenylenyl, dibenzoanthracenyl, fluorenyl, benzofluorenyl, anthracenyl, phenanthrenyl, benzonaphtofuranyl, benzonaphtothiopehnyl, dibenzofuranyl, dibenzothiopehnyl,

[534] which may be each optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40} -

(hetero)alkyl.

[535] In one embodiment, H^{TTA} is an anthracene derivate of the following formula 4, wherein both Ar are residues each independently from each other selected from the group consisting of phenyl, naphthyl, phenanthryl, pyrenyl, triphenylenyl, dibenzoanthracenyl, fluorenyl, benzofluorenyl, anthracenyl, phenanthrenyl, benzonaphtofuranyl, benzonaphtothiopehnyl, dibenzofuranyl, dibenzothiopehnyl,

[536] which may be each optionally substituted with one or more residues selected from the group consisting of C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, halogen, and C_1-C_{40} -(hetero)alkyl.

[537] Compositions comprising an organic molecule according to the invention

[538] One aspect of the invention relates to a composition comprising at least an organic molecule according to the invention. One aspect of the invention relates to the use of this composition in optoelectronic devices, preferably OLEDs, in particular in an EML of said devices.

[539] In the following, when describing the aforementioned composition, reference is in some cases made to the content of certain materials in the respective compositions in form of percentages. It is to be noted that, unless stated otherwise for specific embodiments, all percentages refer to weight percentages, which has the same meaning as percent by weight or % by weight ((weight/weight), (w/w), wt.%). It is understood that, when for example stating that the content of one or more organic molecules according to the invention in a specific composition is exemplarily 30%, this is to mean that the total weight of the one or more organic molecules according to the invention (i.e. of all of these molecules combined) is 30% by weight, i.e. accounts for 30% of the total weight of the respective composition. It is understood that, whenever a composition is specified by providing the preferred content of its components in % by weight, the total content of all components adds up to 100% by weight (i.e. the total weight of the composition).

[540] When in the following describing the embodiments of the invention relating to a composition comprising at least one organic molecule according to the invention, reference will be made to energy transfer processes that may take place between components within these compositions when using said compositions in an optoelectronic device, preferably in an EML of an optoelectronic device, most preferably in an EML of an OLED. The person skilled in the art understands that such excitation energy transfer processes may enhance the emission efficiency when using the composition in an EML of an optoelectronic device.

[541] When describing compositions comprising at least one organic molecule according to the present inventions, it will also be pointed out that certain materials "differ" from other materials. This is to mean the materials that "differ" from each other do not have

the same chemical structure.

[542] In one embodiment, the composition comprises or consists of:

[543] (a) one or more organic molecules according to the invention, and

[544] (b) one or more host materials H^B, which differ from the organic molecules of (a), and

[545] (c) optionally, one or more solvents.

[546] In one embodiment, the composition comprises or consists of:

[547] (a) one or more organic molecules according to the invention, and

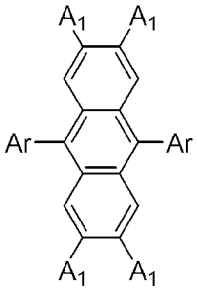
[548] (b) one or more host materials H^B, which differ from the organic molecules of (a),

[549] wherein the fraction of the host materials H^B in % by weight in the composition is higher than the fraction of the organic molecules according to the invention in % by weight, preferably the fraction of the host materials H^B in % by weight in the composition is more than two times higher than the fraction of the organic molecules according to the invention in % by weight.

[550] In one embodiment, the composition comprises or consists of:

[551] (a) 0.1--30% by weight, preferably 0.8--15% by weight, in particular 1.5-5% by weight, of organic molecules according to the invention, and

[552] (b) TTA materials as host materials H^B according to following formula 4:

[553] 

[554] Formula 4.

[555] In one embodiment, the composition comprises or consists of:

[556] (a) organic molecules according to the invention, and

[557] (b) host material H^B, which differ from the organic molecules of (a),

[558] (c) TADF material E^B and/or phosphorescence material P^B.

[559] In one embodiment, the composition comprises or consists of:

[560] (a) 0.1--20% by weight, preferably 0.5-12% by weight, in particular 1-5% by weight of organic molecules according to the invention, and

[561] (b) 0--98.8% by weight, preferably 35--94% by weight, in particular 60--88% by weight of one or more host materials H^B, which differ from the organic molecules according to the invention, and

[562] (c) 0.1--20% by weight, preferably 0.5-10% by weight, in particular 1-3% by weight, of one or more phosphorescence materials P^B, which differ from the organic molecules

of (a), and

[563] (d) 1--99.8% by weight, preferably 5--50% by weight, in particular 10-30% by weight, of one or more TADF materials E^B, which differ from the organic molecules of (a), and

[564] (e) 0--98.8% by weight, preferably 0--59% by weight, in particular 0--28% by weight of one or more solvents.

[565] In a further aspect, the invention relates to an optoelectronic device comprising an organic molecule or a composition of the type described here, more particularly in the form of a device selected from the group consisting of organic light-emitting diode (OLED), light-emitting electrochemical cell, OLED sensor, more particularly gas and vapour sensors not hermetically externally shielded, organic diode, organic solar cell, organic transistor, organic field-effect transistor, organic laser and down-conversion element.

[566] In a preferred embodiment, the optoelectronic device is a device selected from the group consisting of an organic light emitting diode (OLED), a light emitting electro-chemical cell (LEC), and a light-emitting transistor.

[567] In one embodiment of the optoelectronic device of the invention, the organic molecule according to the invention E is used as emission material in a light-emitting layer EML.

[568] In one embodiment of the optoelectronic device of the invention, the light-emitting layer EML consists of the composition according to the invention described here.

[569] When the optoelectronic device is an OLED, it may, for example, have the following layer structure:

[570] 1. substrate

[571] 2. anode layer A

[572] 3. hole injection layer, HIL

[573] 4. hole transport layer, HTL

[574] 5. electron blocking layer, EBL

[575] 6. emitting layer, EML

[576] 7. hole blocking layer, HBL

[577] 8. electron transport layer, ETL

[578] 9. electron injection layer, EIL

[579] 10. cathode layer,

[580] wherein the OLED comprises each layer selected from the group of HIL, HTL, EBL, HBL, ETL, and EIL only optionally, different layers may be merged and the OLED may comprise more than one layer of each layer type defined above.

[581] Furthermore, the optoelectronic device may, in one embodiment, comprise one or more protective layers protecting the device from damaging exposure to harmful

species in the environment including, for example, moisture, vapor and/or gases.

[582] In one embodiment of the invention, the optoelectronic device is an OLED, with the following inverted layer structure:

[583] 1. substrate

[584] 2. cathode layer

[585] 3. electron injection layer, EIL

[586] 4. electron transport layer, ETL

[587] 5. hole blocking layer, HBL

[588] 6. emitting layer, B

[589] 7. electron blocking layer, EBL

[590] 8. hole transport layer, HTL

[591] 9. hole injection layer, HIL

[592] 10. anode layer A

[593] wherein the OLED comprises each layer selected from the group of HIL, HTL, EBL, HBL, ETL, and EIL only optionally, different layers may be merged and the OLED may comprise more than one layer of each layer types defined above.

[594] In one embodiment of the invention, the optoelectronic device is an OLED, which may have a stacked architecture. In this architecture, contrary to the typical arrangement in which the OLEDs are placed side by side, the individual units are stacked on top of each other. Blended light may be generated with OLEDs exhibiting a stacked architecture, in particular white light may be generated by stacking blue, green and red OLEDs. Furthermore, the OLED exhibiting a stacked architecture may comprise a charge generation layer (CGL), which is typically located between two OLED subunits and typically consists of a n-doped and p-doped layer with the n-doped layer of one CGL being typically located closer to the anode layer.

[595] In one embodiment of the invention, the optoelectronic device is an OLED, which comprises two or more emission layers between anode and cathode. In particular, this so-called tandem OLED comprises three emission layers, wherein one emission layer emits red light, one emission layer emits green light and one emission layer emits blue light, and optionally may comprise further layers such as charge generation layers, blocking or transporting layers between the individual emission layers. In a further embodiment, the emission layers are adjacently stacked. In a further embodiment, the tandem OLED comprises a charge generation layer between each two emission layers. In addition, adjacent emission layers or emission layers separated by a charge generation layer may be merged.

[596] The substrate may be formed by any material or composition of materials. Most frequently, glass slides are used as substrates. Alternatively, thin metal layers (e.g., copper, gold, silver or aluminum films) or plastic films or slides may be used. This

may allow for a higher degree of flexibility. The anode layer A is mostly composed of materials allowing to obtain an (essentially) transparent film. As at least one of both electrodes should be (essentially) transparent in order to allow light emission from the OLED, either the anode layer A or the cathode layer C is transparent. Preferably, the anode layer A comprises a large content or even consists of transparent conductive oxides (TCOs). Such anode layer A may, for example, comprise indium tin oxide, aluminum zinc oxide, fluorine doped tin oxide, indium zinc oxide, PbO, SnO, zirconium oxide, molybdenum oxide, vanadium oxide, tungsten oxide, graphite, doped Si, doped Ge, doped GaAs, doped polyaniline, doped polypyrrol and/or doped poly-thiophene.

[597] The anode layer A (essentially) may consist of indium tin oxide (ITO) (e.g., $(InO_3)_{0.9}(SnO_2)_{0.1}$). The roughness of the anode layer A caused by the transparent conductive oxides (TCOs) may be compensated by using a hole injection layer (HIL). Further, the HIL may facilitate the injection of quasi charge carriers (i.e., holes) in that the transport of the quasi charge carriers from the TCO to the hole transport layer (HTL) is facilitated. The hole injection layer (HIL) may comprise poly-3,4-ethylendioxy thiophene (PEDOT), polystyrene sulfonate (PSS), MoO_2, V_2O_5, CuPC or CuI, in particular a mixture of PEDOT and PSS. The hole injection layer (HIL) may also prevent the diffusion of metals from the anode layer A into the hole transport layer (HTL). The HIL may, for example, comprise PEDOT:PSS (poly-3,4-ethylendioxy thiophene: polystyrene sulfonate), PEDOT (poly-3,4-ethylendioxy thiophene), mMTDATA (4,4',4''-tris[phenyl(m-tolyl)amino]triphenylamine), Spiro-TAD (2,2',7,7'-tetrakis(n,n-diphenylamino)-9,9'-spirobifluorene), DNTPD (N1,N1'-(biphenyl-4,4'-diyl)bis(N1-phenyl-N4,N4-di-m-tolylbenzene-1,4-diamine), NPB (N,N'-nis-(1-naphthalenyl)-N,N'-bis-phenyl-(1,1'-biphenyl)-4,4'-diamine), NPNPB (N,N'-diphenyl-N,N'-di-[4-(N,N-diphenyl-amino)phenyl]benzidine), MeO-TPD (N,N,N',N'-tetrakis(4-methoxyphenyl)benzidine), HAT-CN (1,4,5,8,9,11-hexaazatriphenylen-hexacarbonitrile) and/or Spiro-NPD (N,N'-diphenyl-N,N'-bis-(1-naphthyl)-9,9'-spirobifluorene-2,7-diamine).

[598] Adjacent to the anode layer A or the hole injection layer (HIL), a hole transport layer (HTL) is typically located. Herein, any hole transport compound may be used. For example, electron-rich heteroaromatic compounds such as triarylamines and/or carbazoles may be used as hole transport compound. The HTL may decrease the energy barrier between the anode layer A and the light-emitting layer EML. The hole transport layer (HTL) may also be an electron blocking layer (EBL). Preferably, hole transport compounds bear comparably high energy levels of their triplet states T1. For example, the hole transport layer (HTL) may comprise a star-shaped heterocycle such as tris(4-carbazoyl-9-ylphenyl)amine (TCTA), poly-TPD

(poly(4-butylphenyl-diphenyl-amine)), [alpha]-NPD (poly(4-butylphenyl-diphenyl-amine)), TAPC (4,4'-cyclohexyliden-bis[N,N-bis(4-methylphenyl)benzenamine]), 2-TNATA (4,4',4''-tris[2-naphthyl(phenyl)amino]triphenylamine), Spiro-TAD, DNTPD, NPB, NPNPB, MeO-TPD, HAT-CN and/or TrisPcz (9,9'-diphenyl-6-(9-phenyl-9H-carbazol-3-yl)-9H,9'H-3,3'-bicarbazole). In addition, the HTL may comprise a p-doped layer, which may be composed of an inorganic or organic dopant in an organic hole-transporting matrix. Transition metal oxides as vanadium oxide, molybdenum oxide or tungsten oxide may, for example, be used as inorganic dopant. Tetrafluorotetracyanoquinodimethane (F_4-TCNQ), copper-pentafluorobenzoate (Cu(I)pFBz) or transition metal complexes may, for example, be used as organic dopant.

[599] The EBL may, for example, comprise mCP (1,3-bis(carbazol-9-yl)benzene), TCTA, 2-TNATA, mCBP (3,3-di(9H-carbazol-9-yl)biphenyl), tris-Pcz, CzSi (9-(4-tert-butylphenyl)-3,6-bis(triphenylsilyl)-9H-carbazole), and/or DCB (N,N'-dicarbazolyl-1,4-dimethylbenzene).

[600] Adjacent to the hole transport layer (HTL), the light-emitting layer EML is typically located. The light-emitting layer EML comprises at least one light emitting molecule. Particularly, the EML comprises at least one light emitting molecule according to the invention E. In one embodiment, the light-emitting layer comprises only the organic molecules according to the invention. Typically, the EML additionally comprises one or more host materials H. For example, the host material H is selected from CBP (4,4'-Bis-(N-carbazolyl)-biphenyl), mCP, mCBP Sif87 (dibenzo[b,d]thiophen-2-yltriphenylsilane), CzSi, Sif88 (dibenzo[b,d]thiophen-2-yl)diphenylsilane), DPEPO (bis[2-(diphenylphosphino)phenyl] ether oxide), 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzothiophen-2-yl)phenyl]-9H-carbazole, 9-[3,5-bis(2-dibenzofuranyl)phenyl]-9H-carbazole, 9-[3,5-bis(2-dibenzothiophenyl)phenyl]-9H-carbazole, T2T (2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine), T3T (2,4,6-tris(triphenyl-3-yl)-1,3,5-triazine) and/or TST (2,4,6-tris(9,9'-spirobifluorene-2-yl)-1,3,5-triazine). The host material H typically should be selected to exhibit first triplet (T1) and first singlet (S1) energy levels, which are energetically higher than the first triplet (T1) and first singlet (S1) energy levels of the organic molecule.

[601] In one embodiment of the invention, the EML comprises a so-called mixed-host system with at least one hole-dominant host and one electron-dominant host. In a

particular embodiment, the EML comprises exactly one light emitting organic molecule according to the invention and a mixed-host system comprising T2T as electron-dominant host and a host selected from CBP, mCP, mCBP, 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzothiophen-2-yl)phenyl]-9H-carbazole, 9-[3,5-bis(2-dibenzofuranyl)phenyl]-9H-carbazole and 9-[3,5-bis(2-dibenzothiophenyl)phenyl]-9H-carbazole as hole-dominant host. In a further embodiment the EML comprises 50-80 % by weight, preferably 60-75 % by weight of a host selected from CBP, mCP, mCBP, 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzofuran-2-yl)phenyl]-9H-carbazole, 9-[3-(dibenzothiophen-2-yl)phenyl]-9H-carbazole, 9-[3,5-bis(2-dibenzofuranyl)phenyl]-9H-carbazole and 9-[3,5-bis(2-dibenzothiophenyl)phenyl]-9H-carbazole; 10-45 % by weight, preferably 15-30 % by weight of T2T and 5-40 % by weight, preferably 10-30 % by weight of light emitting molecule according to the invention.

[602] Adjacent to the light-emitting layer EML, an electron transport layer (ETL) may be located. Herein, any electron transporter may be used. Exemplarily, electron-poor compounds such as, e.g., benzimidazoles, pyridines, triazoles, oxadiazoles (e.g., 1,3,4-oxadiazole), phosphinoxides and sulfone, may be used. An electron transporter may also be a star-shaped heterocycle such as 1,3,5-tri(1-phenyl-1H-benzo[d]imidazol-2-yl)phenyl (TPBi). The ETL may comprise NBphen (2,9-bis(naphthalen-2-yl)-4,7-diphenyl-1,10-phenanthroline), Alq_3 (Aluminum-tris(8-hydroxyquinoline)), TSPO1 (diphenyl-4-triphenylsilylphenyl-phosphinoxide), BPyTP2 (2,7-di(2,2'-bipyridin-5-yl)triphenyle), Sif87 (dibenzo[b,d]thiophen-2-yltriphenylsilane), Sif88 (dibenzo[b,d]thiophen-2-yl)diphenylsilane), BmPyPhB (1,3-bis[3,5-di(pyridin-3-yl)phenyl]benzene) and/or BTB (4,4′-bis-[2-(4,6-diphenyl-1,3,5-triazinyl)]-1,1′-biphenyl). Optionally, the ETL may be doped with materials as Liq. The transport layer (ETL) may also block holes or a hole-blocking layer (HBL) is introduced.

[603] The HBL may, for example, comprise BCP (2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline = Bathocuproine), BAlq (bis(8-hydroxy-2-methylquinoline)-(4-phenylphenoxy)aluminum), NBphen (2,9-bis(naphthalen-2-yl)-4,7-diphenyl-1,10-phenanthroline), Alq_3 (Aluminum-tris(8-hydroxyquinoline)), TSPO1

(diphenyl-4-triphenylsilylphenyl-phosphinoxide), T2T (2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine), T3T (2,4,6-tris(triphenyl-3-yl)-1,3,5-triazine), TST (2,4,6-tris(9,9′-spirobifluorene-2-yl)-1,3,5-triazine), and/or TCB/TCP (1,3,5-tris(N-carbazolyl)benzol/ 1,3,5-tris(carbazol)-9-yl) benzene).

[604] Adjacent to the electron transport layer (ETL), a cathode layer C may be located.The cathode layer C may, for example, comprise or may consist of a metal (e.g., Al, Au, Ag, Pt, Cu, Zn, Ni, Fe, Pb, LiF, Ca, Ba, Mg, In, W, or Pd) or a metal alloy. For practical reasons, the cathode layer may also consist of (essentially) intransparent metals such as Mg, Ca or Al. Alternatively or additionally, the cathode layer C may also comprise graphite and/or carbon nanotubes (CNTs). Alternatively, the cathode layer C may also consist of nanoscalic silver wires.

[605] An OLED may further, optionally, comprise a protection layer between the electron transport layer (ETL) and the cathode layer C (which may be designated as electron injection layer (EIL)). This layer may comprise lithium fluoride, cesium fluoride, silver, Liq (8-hydroxyquinolinolatolithium), Li_2O, BaF_2, MgO and/or NaF.

[606] Optionally, the electron transport layer (ETL) and/or a hole blocking layer (HBL) may also comprise one or more host compounds H.

[607] In order to modify the emission spectrum and/or the absorption spectrum of the light-emitting layer EML further, the light-emitting layer EML may further comprise one or more further emitter molecules F. Such an emitter molecule F may be any emitter molecule known in the art. Preferably such an emitter molecule F is a molecule with a structure differing from the structure of the molecules according to the invention E. The emitter molecule F may optionally be a TADF emitter. Alternatively, the emitter molecule F may optionally be a fluorescent and/or phosphorescent emitter molecule which is able to shift the emission spectrum and/or the absorption spectrum of the light-emitting layer EML. Exemplarily, the triplet and/or singlet excitons may be transferred from the organic emitter molecule according to the invention to the emitter molecule F before relaxing to the ground state S0 by emitting light typically red-shifted in comparison to the light emitted by an organic molecule. Optionally, the emitter molecule F may also provoke two-photon effects (i.e., the absorption of two photons of half the energy of the absorption maximum).

[608] Optionally, an optoelectronic device (e.g., an OLED) may, for example, be an essentially white optoelectronic device. For example, such a white optoelectronic device may comprise at least one (deep) blue emitter molecule and one or more emitter molecules emitting green and/or red light. Then, there may also optionally be energy transmittance between two or more molecules as described above.

[609] As used herein, if not defined more specifically in the particular context, the designation of the colors of emitted and/or absorbed light is as follows:

[610] violet: wavelength range of >380-420 nm;

[611] deep blue: wavelength range of >420-480 nm;

[612] sky blue: wavelength range of >480-500 nm;

[613] green: wavelength range of >500-560 nm;

[614] yellow: wavelength range of >560-580 nm;

[615] orange: wavelength range of >580-620 nm;

[616] red: wavelength range of >620-800 nm.

[617] With respect to emitter molecules, such colors refer to the emission maximum. Therefore, for example, a deep blue emitter has an emission maximum in the range of from >420 to 480 nm, a sky blue emitter has an emission maximum in the range of from >480 to 500 nm, a green emitter has an emission maximum in a range of from >500 to 560 nm, a red emitter has an emission maximum in a range of from >620 to 800 nm.

[618] A deep blue emitter may preferably have an emission maximum of below 480 nm, more preferably below 470 nm, even more preferably below 465 nm or even below 460 nm. It will typically be above 420 nm, preferably above 430 nm, more preferably above 440 nm or even above 450 nm.

[619] A green emitter has an emission maximum of below 560 nm, more preferably below 550 nm, even more preferably below 545 nm or even below 540 nm. It will typically be above 500 nm, more preferably above 510 nm, even more preferably above 515 nm or even above 520 nm.

[620] Accordingly, a further aspect of the present invention relates to an OLED, which exhibits an external quantum efficiency at 1000 cd/m^2 of more than 8 %, more preferably of more than 10 %, more preferably of more than 13 %, even more preferably of more than 15 % or even more than 20 % and/or exhibits an emission maximum between 420 nm and 500 nm, preferably between 430 nm and 490 nm, more preferably between 440 nm and 480 nm, even more preferably between 450 nm and 470 nm and/or exhibits a LT80 value at 500 cd/m^2 of more than 100 h, preferably more than 200 h, more preferably more than 400 h, even more preferably more than 750 h or even more than 1000 h. Accordingly, a further aspect of the present invention relates to an OLED, whose emission exhibits a CIEy color coordinate of less than 0.45, preferably less than 0.30, more preferably less than 0.20 or even more preferably less than 0.15 or even less than 0.10.

[621] A further aspect of the present invention relates to an OLED, which emits light with CIEx and CIEy color coordinates close to the CIEx (= 0.170) and CIEy (= 0.797) color coordinates of the primary color green (CIEx = 0.170 and CIEy = 0.797) as defined by ITU-R Recommendation BT.2020 (Rec. 2020) and thus is suited for the use in Ultra High Definition (UHD) displays, e.g. UHD-TVs. In this context, the term "close to"

refers to the ranges of CIEx and CIEy coordinates provided at the end of this paragraph. In commercial applications, typically top-emitting (top-electrode is transparent) devices are used, whereas test devices as used throughout the present application represent bottom-emitting devices (bottom-electrode and substrate are transparent). Accordingly, a further aspect of the present invention relates to an OLED, whose emission exhibits a CIEx color coordinate of between 0.15 and 0.45 preferably between 0.15 and 0.35, more preferably between 0.15 and 0.30 or even more preferably between 0.15 and 0.25 or even between 0.15 and 0.20 and/ or a CIEy color coordinate of between 0.60 and 0.92, preferably between 0.65 and 0.90, more preferably between 0.70 and 0.88 or even more preferably between 0.75 and 0.86 or even between 0.79 and 0.84.

[622] Accordingly, a further aspect of the present invention relates to an OLED, which exhibits an external quantum efficiency at 14500 cd/m^2 of more than 8%, more preferably of more than 10%, more preferably of more than 13%, even more preferably of more than 15% or even more than 17%, or even more than 20% and/or exhibits an emission maximum between 485 nm and 560 nm, preferably between 500 nm and 560 nm, more preferably between 510 nm and 550 nm, even more preferably between 515 nm and 540 nm and/or exhibits a LT97 value at 14500 cd/m^2 of more than 100 h, preferably more than 250 h, more preferably more than 50 h, even more preferably more than 750 h or even more than 1000 h.

[623] A further aspect of the present invention relates to an OLED, which emits light at a distinct color point. According to the present invention, the OLED emits light with a narrow emission band (small full width at half maximum (FWHM)). In one aspect, the OLED according to the invention emits light with a FWHM of the main emission peak of less than 0.25 eV, preferably less than 0.20 eV, more preferably less than 0.17 eV, even more preferably less than 0.15 eV or even less than 0.13 eV.

[624] In a further embodiment of the invention, the composition has a photoluminescence quantum yield (PLQY) of more than 20 %, preferably more than 30 %, more preferably more than 35 %, more preferably more than 40 %, more preferably more than 45 %, more preferably more than 50 %, more preferably more than 55 %, even more preferably more than 60 % or even more than 70 % at room temperature.

[625] In a further aspect, the invention relates to a method for producing an optoelectronic component. In this case an organic molecule of the invention is used.

[626] In a further aspect, the invention relates to a method for generating light at a wavelength range from 510 nm to 550 nm, preferably from 520 nm to 540 nm, comprising the steps of:

[627] (i) providing an optoelectronic device comprising an organic molecule of the invention and

[628] (ii) applying an electrical current to said electroluminescent device.

[629] The optoelectronic device, in particular the OLED according to the present invention can be fabricated by any means of vapor deposition and/ or liquid processing. Accordingly, at least one layer is

[630] - prepared by means of a sublimation process,

[631] - prepared by means of an organic vapor phase deposition process,

[632] - prepared by means of a carrier gas sublimation process or

[633] - solution processed or printed.

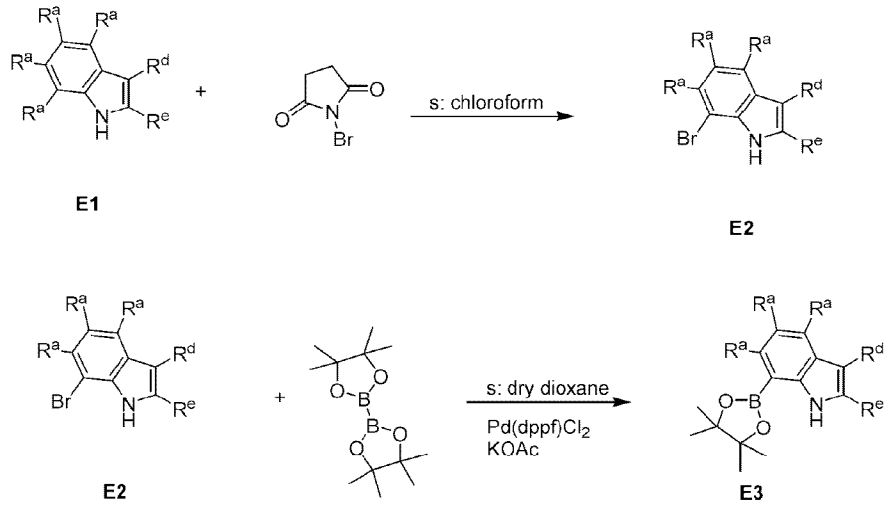
[634] The methods used to fabricate the optoelectronic device, in particular the OLED according to the present invention are known in the art. The different layers are individually and successively deposited on a suitable substrate by means of subsequent deposition processes. The individual layers may be deposited using the same or differing deposition methods.

[635] Vapor deposition processes, for example, comprise thermal (co)evaporation, chemical vapor deposition and physical vapor deposition. For active matrix OLED display, an AMOLED backplane is used as substrate. The individual layer may be processed from solutions or dispersions employing adequate solvents. Solution deposition process, for example, comprise spin coating, dip coating and jet printing. Liquid processing may optionally be carried out in an inert atmosphere (e.g., in a nitrogen atmosphere) and the solvent may be completely or partially removed by means known in the state of the art.

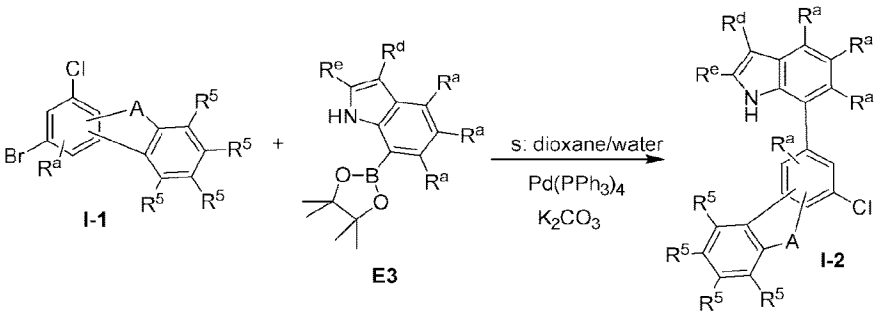
[636] Examples

[637] **General synthesis scheme I**

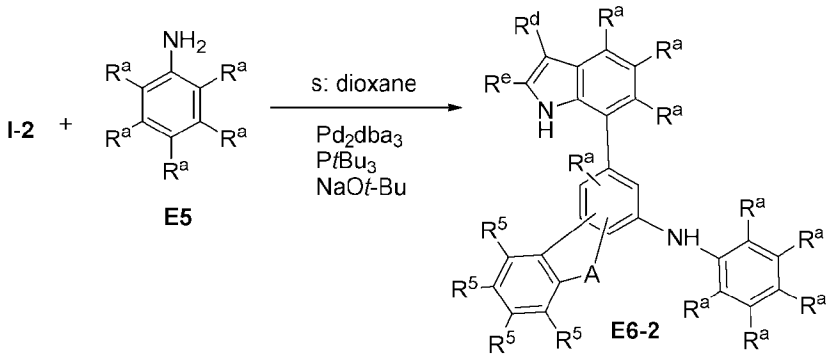
[638] (exemplified for Z = direct bond, whereby the following synthesis schemes can also be applied for Z being different to a direct bond)

[639] 

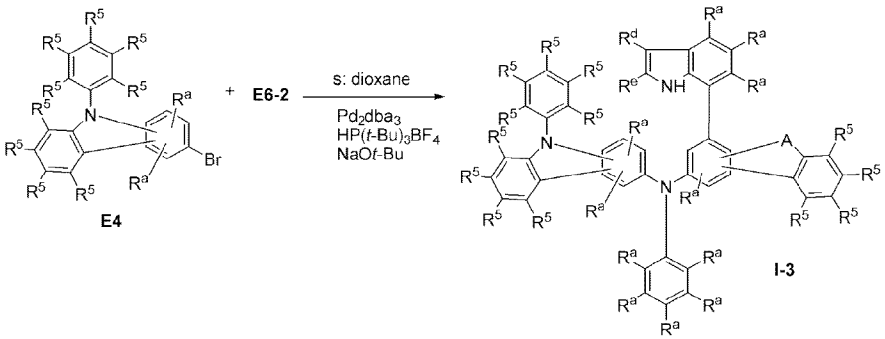
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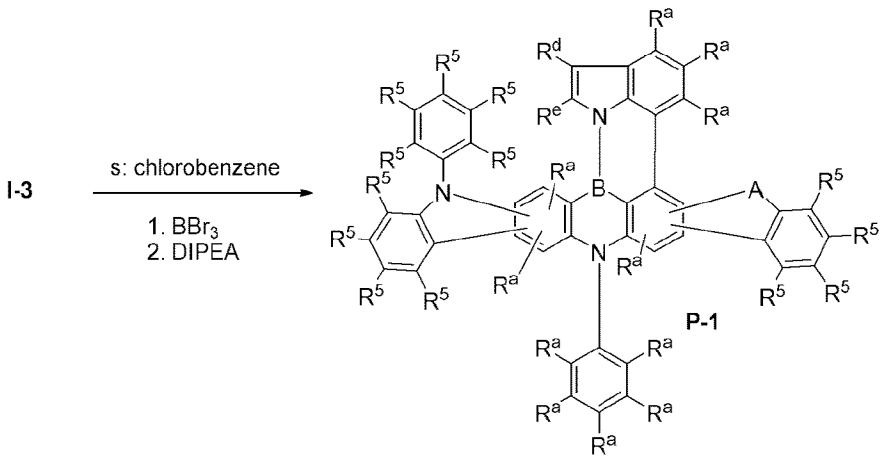
[641]



[642]



[643]



[644] *General procedure for synthesis:*

[645] **AAV1:**

[646] E1 (1.00 equivalents) is solved in dry chloroform and N-bromosuccinimide (CAS: 128-08-5, 1.05 equivalents) is added in portions under nitrogen atmosphere at 0 °C. The mixture is stirred at room temperature for 2 h and subsequently extracted between

chloroform and water and the combined organic layers concentrated under reduced pressure. The crude is purified by column chromatography or recrystallization and **E2** is obtained as a solid.

[647] **AAV2:**

[648] E2 (1.00 equivalents), bis(pinacolato)diboron (CAS: 73183-34-3, 1.5 equivalents), [1,1'-bis(diphenylphosphino)ferrocene]palladium (II) dichloride (CAS: 72287-26-4, 0.02 equivalents) and potassium acetate (KOAc; CAS: 127-08-2, 3.00 equivalents) are stirred under nitrogen atmosphere in dry dioxane at 95 °C for 24 h. After cooling down to room temperature (rt) the reaction mixture is extracted between dichloromethane and water and the combined organic layers concentrated under reduced pressure. The crude is purified by column chromatography or recrystallization and **E3** is obtained as a solid.

[649] **AAV3:**

[650] E3 (1.00 equivalents), **I-1** (1.05 equivalents), tetrakis(triphenylphosphine)palladium(0) (CAS: 14221-01-3, 0.05 equivalents) and potassium carbonate (K_2CO_3; CAS: 584-08-7, 2.00 equivalents) are stirred under nitrogen atmosphere in dioxane/water (10:1 by vol.) at 80 °C until completion of the reaction (TLC control). After cooling down to room temperature (rt) the reaction mixture is extracted between ethyl acetate and water and the combined organic layers concentrated under reduced pressure. The crude is purified by column chromatography or recrystallization and **I-2** is obtained as a solid.

[651] **AAV4:**

[652] **I-2** (1.00 equivalents), **E5** (1.60 equivalents), tris(dibenzylideneacetone)-dipalladium(0) (CAS: 51364-51-3 , 0.02 equivalents), sodium tert-butoxide (NaOtBu, CAS: 865-48-5, 2.40 equivalents) and tri-tert-butylphosphine (Pt-Bu_3; CAS: 13716-12-6, 0.08 equivalents) are stirred under nitrogen atmosphere in dry dioxane at 95 °C until completion of the reaction (TLC control). After cooling down to room temperature (rt) the reaction mixture is extracted between ethyl acetate and brine and the combined organic layers concentrated under reduced pressure. The crude material is purified by column chromatography or by re-crystallization and **E6-2** is obtained as solid.

[653] **AAV5:**

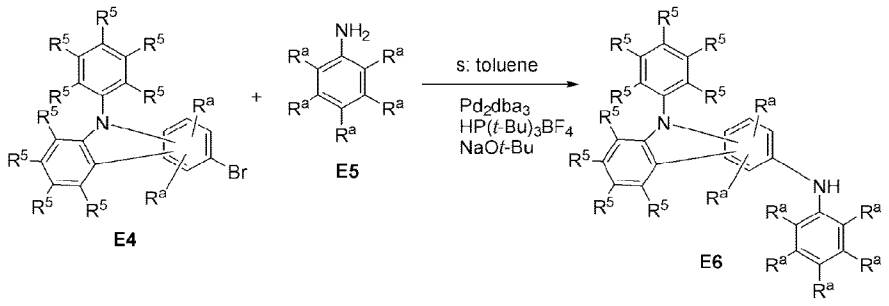
[654] E6-2 (1.00 equivalents), **E4** (1.12 equivalents), tris(dibenzylideneacetone)-dipalladium(0) (CAS: 51364-51-3 , 0.015 equivalents), sodium tert-butoxide (NaOtBu, CAS: 865-48-5, 2.20 equivalents) and tri-tert-butylphosphonium tetrafluoroborate ($HP(t\text{-}Bu)_3BF_4$; CAS: 131274-22-1, 0.06 equivalents) are stirred under nitrogen atmosphere in dry dioxane at 80 °C until completion of the reaction (TLC control). After cooling down to room temperature (rt)

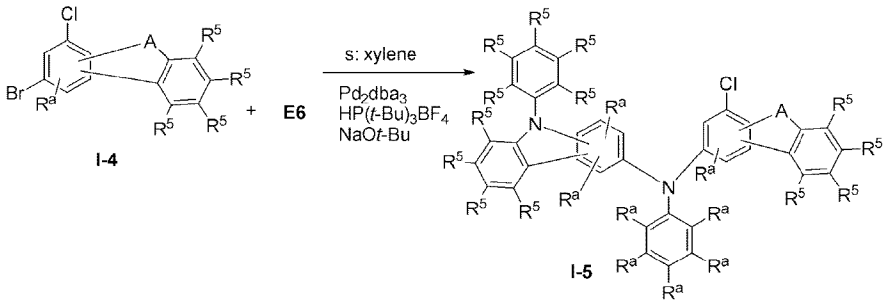
the reaction mixture is extracted between ethyl acetate and brine and the combined organic layers concentrated under reduced pressure. The crude material is purified by column chromatography or by recrystallization and **I-3** is obtained as solid.

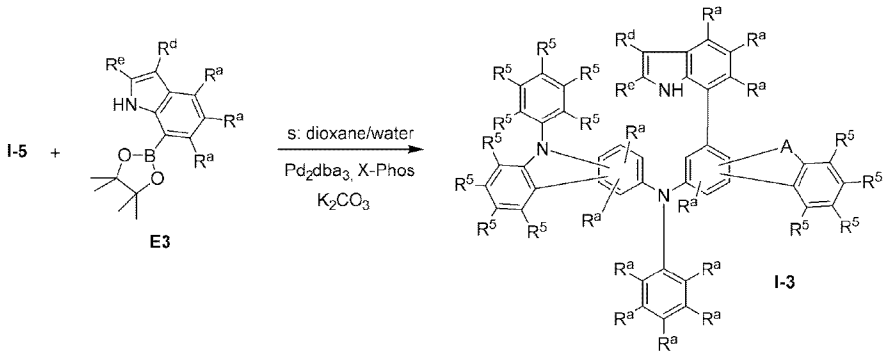
[655] **AAV6:**

[656] Under nitrogen in dry chlorobenzene, **I-3** (1.00 equivalents) is reacted with BBr_3 (4.00 equivalents, CAS: 10294-33-4) at -10°C for 1 h, 1 h at rt, 5 h at 60°C. Afterwards, the mixture is cooled down to rt, followed by the addition of DIPEA (10.0 equivalents, CAS: 7087-68-5). Water is added, the phases separated and the aqueous layer extracted with ethyl acetate. The combined organic layers are washed with water, dried over $MgSO_4$, filtered and concentrated. The crude is purified by column chromatography or recrystallization to yield compound **P-1** as a solid.

[657] **General synthesis scheme II**

[658] 

[659] 

[660] 

[661] *General procedure for synthesis:*

[662] **AAV7:**

[663] E4 (1.00 equivalents), **E5** (1.60 equivalents), tris(dibenzylideneacetone)-dipalladium(0) (CAS: 51364-51-3 , 0.005 equivalents), sodium tert-butoxide (NaOtBu, CAS: 865-48-5, 2.10 equivalents) and tri-

tert-butylphosphonium tetrafluoroborate ($HP(t\text{-}Bu)_3BF_4$; CAS: 131274-22-1, 0.02 equivalents) are stirred under nitrogen atmosphere in dry toluene at 60 °C until completion of the reaction (TLC control). After cooling down to room temperature (rt) the reaction mixture is extracted between ethyl acetate and brine and the combined organic layers concentrated under reduced pressure. The crude material is purified by column chromatography or by recrystallization and **E6** is obtained as a solid.

[664] **AAV8:**

[665] I-4 (1.15 equivalents), **E6** (1.00 equivalents), tris(dibenzylideneacetone)-dipalladium(0) (CAS: 51364-51-3 , 0.02 equivalents), sodium tert-butoxide (NaOtBu, CAS: 865-48-5, 2.00 equivalents) and tri-tert-butylphosphonium tetrafluoroborate ($HP(t\text{-}Bu)_3BF_4$; CAS: 131274-22-1, 0.08 equivalents) are stirred under nitrogen atmosphere in dry toluene at 80 °C until completion of the reaction (TLC control). After cooling down to room temperature (rt) the reaction mixture is extracted between ethyl acetate and brine and the combined organic layers concentrated under reduced pressure. The crude material is purified by column chromatography or by recrystallization and **I-5** is obtained as a solid.

[666] **AAV9:**

[667] E3 (1.25 equivalents), **I-5** (1.00 equivalents), Tris(dibenzylideneacetone)-dipalladium(0) (CAS-No. 51364-51-3, 0.04 equivalents), X-Phos (CAS-No. 564483-18-7, 0.16 equivalents) and K_2CO_3 (CAS-No. 584-08-7, 2.50 equivalents) are stirred under nitrogen atmosphere in dioxane/water (10:1 by vol.) at 80 °C until completion of the reaction (TLC control). After cooling down to room temperature (rt) the reaction mixture is extracted between ethyl acetate and water and the combined organic layers concentrated under reduced pressure. The crude material is purified by column chromatography or by recrystallization and **I-3** is obtained as a solid.

[668] *Cyclic voltammetry*

[669] Cyclic voltammograms are measured from solutions having concentration of 10^{-3} mol/L of the organic molecules in dichloromethane or a suitable solvent and a suitable supporting electrolyte (e.g. 0.1 mol/L of tetrabutylammonium hexafluorophosphate). The measurements are conducted at room temperature under nitrogen atmosphere with a three-electrode assembly (Working and counter electrodes: Pt wire, reference electrode: Pt wire) and calibrated using $FeCp_2/FeCp_2^+$ as internal standard. The HOMO data was corrected using ferrocene as internal standard against a saturated calomel electrode (SCE).

[670] *Density functional theory calculation*

[671] Molecular structures are optimized employing the BP86 functional and the resolution of identity approach (RI). Excitation energies are calculated using the (BP86)

optimized structures employing Time-Dependent DFT (TD-DFT) methods. Orbital and excited state energies are calculated with the B3LYP functional. Def2-SVP basis sets (and a m4-grid for numerical integration are used. The Turbomole program package is used for all calculations.

[672] *Photophysical measurements*

[673] Sample pretreatment: Spin-coating

[674] Apparatus: Spin150, SPS euro.

[675] The sample concentration is 10 mg/ml, dissolved in a suitable solvent.

[676] Program: 1) 3 s at 400 U/min; 20 s at 1000 U/min at 1000 Upm/s. 3) 10 s at 4000 U/min at 1000 Upm/s. After coating, the films are tried at 70 °C for 1 min.

[677] Absorption measurements

[678] A Thermo Scientific Evolution 201 UV-Visible Spectrophotometer is used to determine the wavelength of the absorption maximum of the sample in the wavelength region above 270 nm. This wavelength is used as excitation wavelength for photoluminescence spectral and quantum yield measurements.

[679] Photoluminescence spectra

[680] Steady-state emission spectra are recorded using a Horiba Scientific, Modell FluoroMax-4 equipped with a 150 W Xenon-Arc lamp, excitation- and emissions monochromators. The samples are placed in a cuvette and flushed with nitrogen during the measurements.

[681] Photoluminescence spectroscopy and Time-Correlated Single-Photon Counting (TCSPC)

[682] Steady-state emission spectroscopy is measured by a Horiba Scientific, Modell FluoroMax-4 equipped with a 150 W Xenon-Arc lamp, excitation- and emissions monochromators and a Hamamatsu R928 photomultiplier and a time-correlated single-photon counting option. Emissions and excitation spectra are corrected using standard correction fits.

[683] Excited state lifetimes are determined employing the same system using the TCSPC method with FM-2013 equipment and a Horiba Yvon TCSPC hub.

[684] Excitation sources:

[685] NanoLED 370 (wavelength: 371 nm, puls duration: 1,1 ns)

[686] NanoLED 290 (wavelength: 294 nm, puls duration: <1 ns)

[687] SpectraLED 310 (wavelength: 314 nm)

[688] SpectraLED 355 (wavelength: 355 nm).

[689] Data analysis (exponential fit) is done using the software suite DataStation and DAS6 analysis software. The fit is specified using the chi-squared-test.

[690] Photoluminescence quantum yield measurements

[691] For photoluminescence quantum yield (PLQY) measurements an *Absolute PL*

Quantum Yield Measurement C9920-03G system (*Hamamatsu Photonics*) is used. Quantum yields and CIE coordinates are determined using the software U6039-05 version 3.6.0.

[692] Emission maxima are given in nm, quantum yields Φ in % and CIE coordinates as x,y values.

[693] PLQY is determined using the following protocol:

[694] 1) Quality assurance: Anthracene in ethanol (known concentration) is used as reference

[695] 2) Excitation wavelength: the absorption maximum of the organic molecule is determined and the molecule is excited using this wavelength

[696] 3) Measurement

[697] Quantum yields are measured, for sample, of solutions or films under nitrogen atmosphere. The yield is calculated using the equation:

[698] $$\Phi_{PL} = \frac{n_{photon}, emited}{n_{photon}, absorbed} = \frac{\int \frac{\lambda}{hc}\left[Int^{sample}_{emitted}(\lambda) - Int^{sample}_{absorbed}(\lambda)\right]d\lambda}{\int \frac{\lambda}{hc}\left[Int^{reference}_{emitted}(\lambda) - Int^{reference}_{absorbed}(\lambda)\right]d\lambda}$$

[699] wherein n_{photon} denotes the photon count and Int. the intensity.

[700] Production and characterization of optoelectronic devices

[701] Optoelectronic devices, such as OLED devices comprising organic molecules according to the invention can be produced via vacuum-deposition methods. If a layer contains more than one compound, the weight-percentage of one or more compounds is given in %. The total weight-percentage values amount to 100 %, thus if a value is not given, the fraction of this compound equals to the difference between the given values and 100 %.

[702] The not fully optimized OLEDs are characterized using standard methods and measuring electroluminescence spectra, the external quantum efficiency (in %) in dependency on the intensity, calculated using the light detected by the photodiode, and the current. The OLED device lifetime is extracted from the change of the luminance during operation at constant current density. The LT50 value corresponds to the time, where the measured luminance decreased to 50 % of the initial luminance, analogously LT80 corresponds to the time point, at which the measured luminance decreased to 80 % of the initial luminance, LT 95 to the time point, at which the measured luminance decreased to 95 % of the initial luminance etc.

[703] Accelerated lifetime measurements are performed (e.g. applying increased current densities). For example, LT80 values at 500 cd/m^2 are determined using the following equation:

[704] $$\mathrm{LT80}\left(500\frac{cd^2}{m^2}\right) = \mathrm{LT80}(L_0)\left(\frac{L_0}{500\frac{cd^2}{m^2}}\right)^{1.6}$$

[705] wherein L_0 denotes the initial luminance at the applied current density.

[706] The values correspond to the average of several pixels (typically two to eight), the standard deviation between these pixels is given.

[707] **HPLC-MS:**

[708] HPLC-MS analysis is performed on an HPLC by Agilent (1100 series) with MS-detector (Thermo LTQ XL).

[709] Exemplary a typical HPLC method is as follows: a reverse phase column 4,6mm x 150mm, particle size 3,5 µm from Agilent *(ZORBAX Eclipse Plus 95Angstrom C18, 4.6 x 150 mm, 3.5 µm HPLC column)* is used in the HPLC. The HPLC-MS measurements are performed at room temperature (rt) following gradients:

[710] [Table 1]

Flow rate [ml/min]	Time [min]	A[%]	B[%]	C[%]
2.5	0	40	50	10
2.5	5	40	50	10
2.5	25	10	20	70
2.5	35	10	20	70
2.5	35.01	40	50	10
2.5	40.01	40	50	10
2.5	41.01	40	50	10

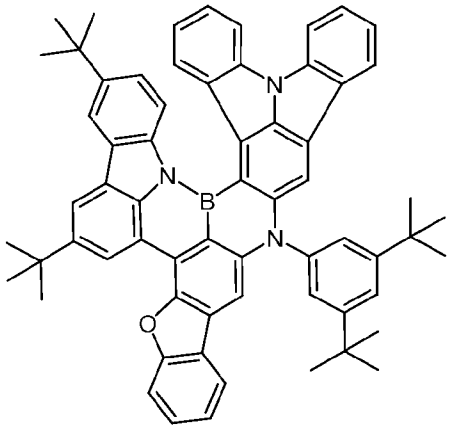
[711] using the following solvent mixtures:

[712] [Table 2]

Solvent A:	H2O (90%)	MeCN (10%)
Solvent B:	H2O (10%)	MeCN (90%)
Solvent C:	THF (50%)	MeCN (50%)

[713] An injection volume of 5 µL from a solution with a concentration of 0.5 mg/mL of the analyte is taken for the measurements.Ionization of the probe is performed using an APCI (atmospheric pressure chemical ionization) source either in positive (APCI +) or negative (APCI -) ionization mode.

[714] **Example 1**

[715] 

[716] Example 1 was synthesized according to

[717] **AAV1** (99% yield), where the starting material **E1** was represented by 3,6-di-tert-butylcarbazole (CAS-no. 37500-95-1);

[718] **AAV2** (63% yield);

[719] **AAV3** (87% yield), where compound **I-1** was represented by 4-bromo-2-chlorodibenzo[b,d]furan (CAS-no. 2087889-86-7);

[720] **AAV4** (47% yield) where starting material **E5** was represented by 3,5-di-tert-butylaniline (CAS-no. 2380-36-1);

[721] **AAV5** (83% yield) where starting material **E4** was represented by 2-broMoindolo[3,2,1-jk]carbazole (CAS-no. 1174032-81-5);

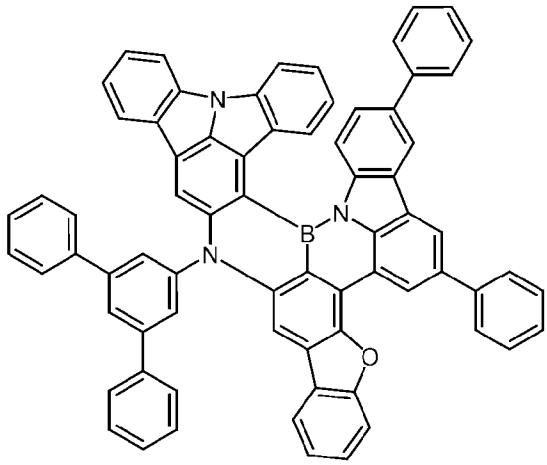
[722] and **AAV6** (49% yield)

[723] MS (LC-MS, APPI ion source): 897 m/z at rt: 9.20 min.

[724] The emission maximum of example **1** (0.001 mg/mL in toluene) is at 520 nm with a full-width at half maximum (FWHM) of 19 nm, the CIEx coordinate is 0.24 and the CIEy coordinate is 0.70. The photoluminescence quantum yield (PLQY) is 69%.

[725] The absorption maximum of example **1** (0.01 mg/mL in toluene) is at 513 nm and has an absorption coefficient at the absorption maximum of 39000 $M^{-1}cm^{-1}$.

[726] **Example 2**

[727] 

[728] Example 2 was synthesized according to

[729] **AAV1** (85% yield), where starting material **E1** was represented by 3,6-diphenylcarbazole (CAS-no. 56525-79-2);

[730] **AAV2** (54% yield);

[731] **AAV7** (38% yield) where starting materials **E4** and **E5** were represented by 2-bromoindolo[3,2,1-jk]carbazole (CAS-no. 1174032-81-5) and 3,5-diphenylaniline (CAS-no. 63006-66-6);

[732] **AAV8** (91% yield) where compound **I-4** was represented by 2-bromo-4-chloro-dibenzofuran (CAS-no. 1960445-63-9);

[733] **AAV9** (66% yield);

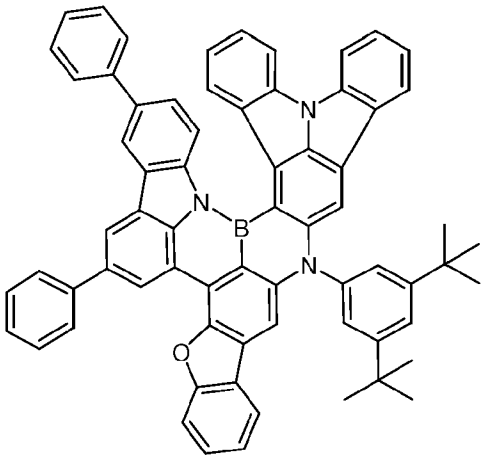
[734] and **AAV6** (19% yield)

[735] MS (LC-MS, APPI ion source): 977 m/z at rt: 10.41 min.

[736] The emission maximum of example **2** (0.001 mg/mL in toluene) is at 521 nm with a full-width at half maximum (FWHM) of 19 nm, the CIEx coordinate is 0.24 and the CIEy coordinate is 0.69. The photoluminescence quantum yield (PLQY) is 80%.

[737] The absorption maximum of example **2** (0.01 mg/mL in toluene) is at 514 nm and has an absorption coefficient at the absorption maximum of 51000 $M^{-1}cm^{-1}$.

[738] **Example 3**

[739] 

[740] Example 3 was synthesized according to

[741] ***AAV1*** (85% yield), where starting material **E1** was represented by 3,6-diphenylcarbazole (CAS-no. 56525-79-2);

[742] ***AAV2*** (54% yield);

[743] ***AAV3*** (56% yield), where compound **I-1** was represented by 4-bromo-2-chlorodibenzo[b,d]furan (CAS-no. 2087889-86-7);

[744] ***AAV4*** (83% yield) where starting material **E5** was represented by 3,5-di-tert-butylaniline (CAS-no. 2380-36-1);

[745] **AAV5** (68% yield) where compound **E4** was represented by 2-bro-moindolo[3,2,1-jk]carbazole (CAS-no. 1174032-81-5);

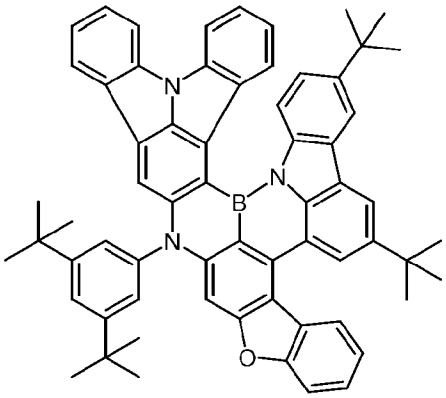
[746] and **AAV6** (32% yield)

[747] MS (LC-MS, APCI ion source): 937 m/z at rt: 8.72 min.

[748] The emission maximum of example **3** (0.001 mg/mL in toluene) is at 524 nm with a full-width at half maximum (FWHM) of 19 nm, the CIEx coordinate is 0.26 and the CIEy coordinate is 0.70. The photoluminescence quantum yield (PLQY) is 80%.

[749] The absorption maximum of example **3** (0.01 mg/mL in toluene) is at 517 nm and has an absorption coefficient at the absorption maximum of 49000 $M^{-1}cm^{-1}$.

[750] **Example 4**

[751] 

[752] Example 4 was synthesized according to

[753] ***AAV1*** (99% yield), where starting material **E1** was represented by 3,6-di-tert-butylcarbazole (CAS-no. 37500-95-1);

[754] ***AAV2*** (63% yield);

[755] ***AAV3*** (16% yield), where compound **I-1** was represented by 1-Bromo-3-chlorodibenzo[b,d]furan (CAS-no. 2043962-13-4);

[756] ***AAV7*** (73% yield) where starting materials **E4** and **E5** were represented by 2-bromoindolo[3,2,1-jk]carbazole (CAS-no. 1174032-81-5) and 3,5-Di-tert-butylaniline (CAS-no. 2380-36-1);

[757] **AAV8** (28% yield);

[758] and **AAV6** (52% yield)

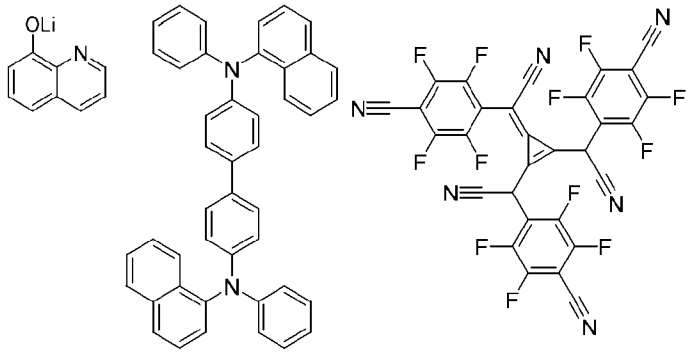
[759] MS (LC-MS, APCI ion source): 897 m/z at rt: 9.31 min.

[760] The emission maximum of example **4** (0.001 mg/mL in toluene) is at 509 nm with a full-width at half maximum (FWHM) of 24 nm, the CIEx coordinate is 0.19 and the CIEy coordinate is 0.65. The photoluminescence quantum yield (PLQY) is 55%.

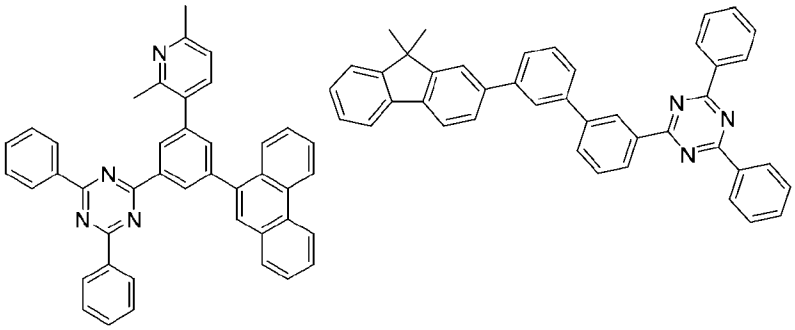
[761] The absorption maximum of example **4** (0.01 mg/mL in toluene) is at 499 nm and has an absorption coefficient at the absorption maximum of 30000 $M^{-1}cm^{-1}$.

[762] **Example OLED Device D1**

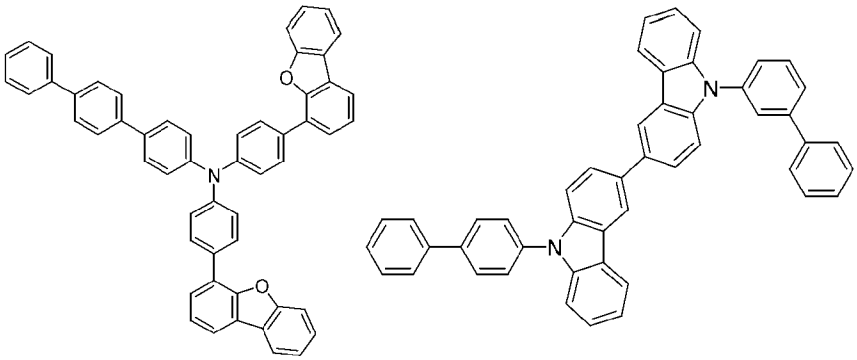
[763] Stack material

[764] 

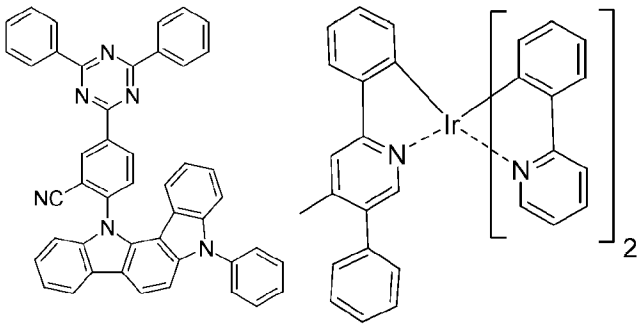
[765] Liq NPB NDP-9

[766] 

[767] ETM1 (electron-transporting material) ETM2 (electron-transporting material)

[768] 

[769] EBM1 (electron-blocking material) Host1 (host material)

[770] 

[771] TADF1 (TADF material) Phos1 (phosphorescence material)

[772] Example **2** was tested in the OLED **D1**, which was fabricated with the following layer structure:

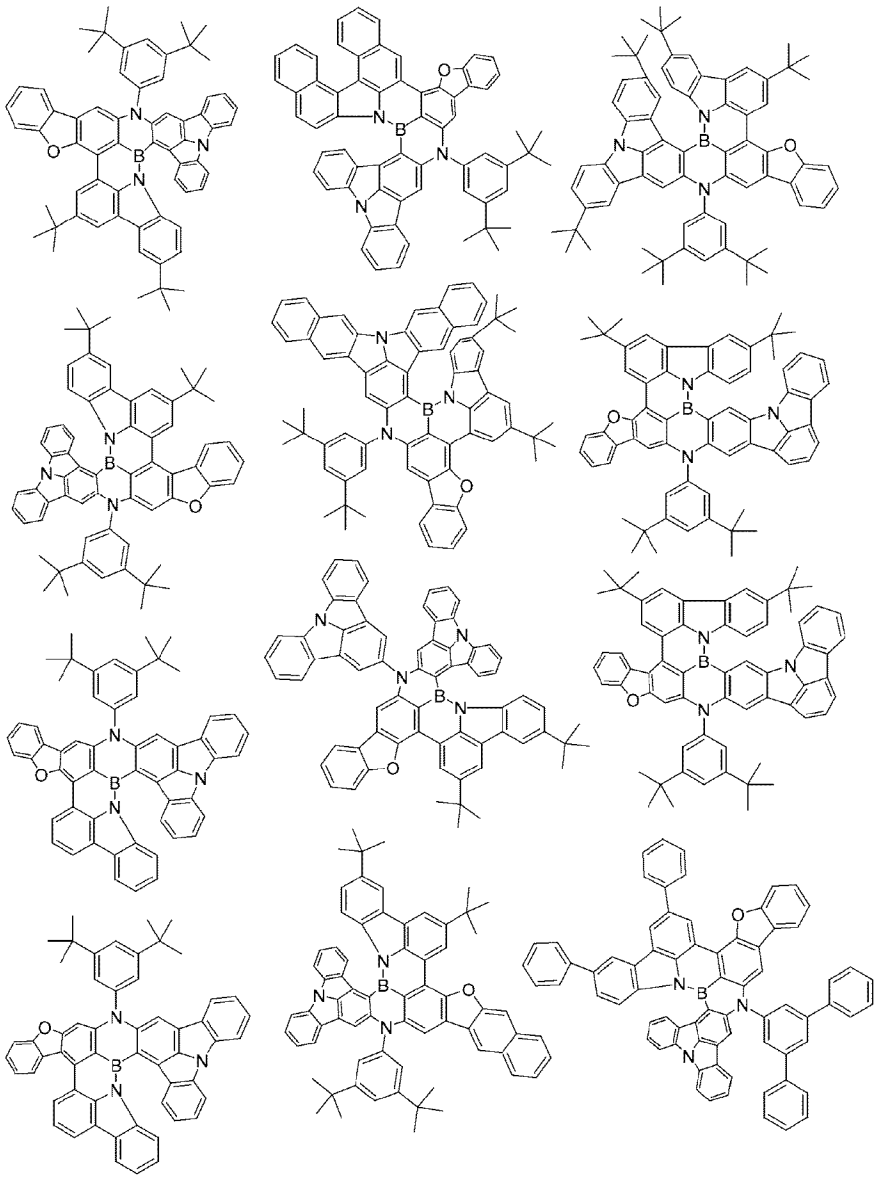
[773] [Table 3]

Layer #	**Thickness**	**D1**
9	100 nm	Al
8	2 nm	Liq
7	27 nm	ETM1 (50%) : Liq (50%)
6	5 nm	ETM2
5	60 nm	Host1 (66.3%) : TADF1 (30%) : Phos1 (3%) : Example **2** (0.7%)
4	10 nm	EBM1
3	44 nm	NPB
2	9 nm	NPB (95%) : NDP-9 (5%)
1	50 nm	ITO
Substrate		Glass

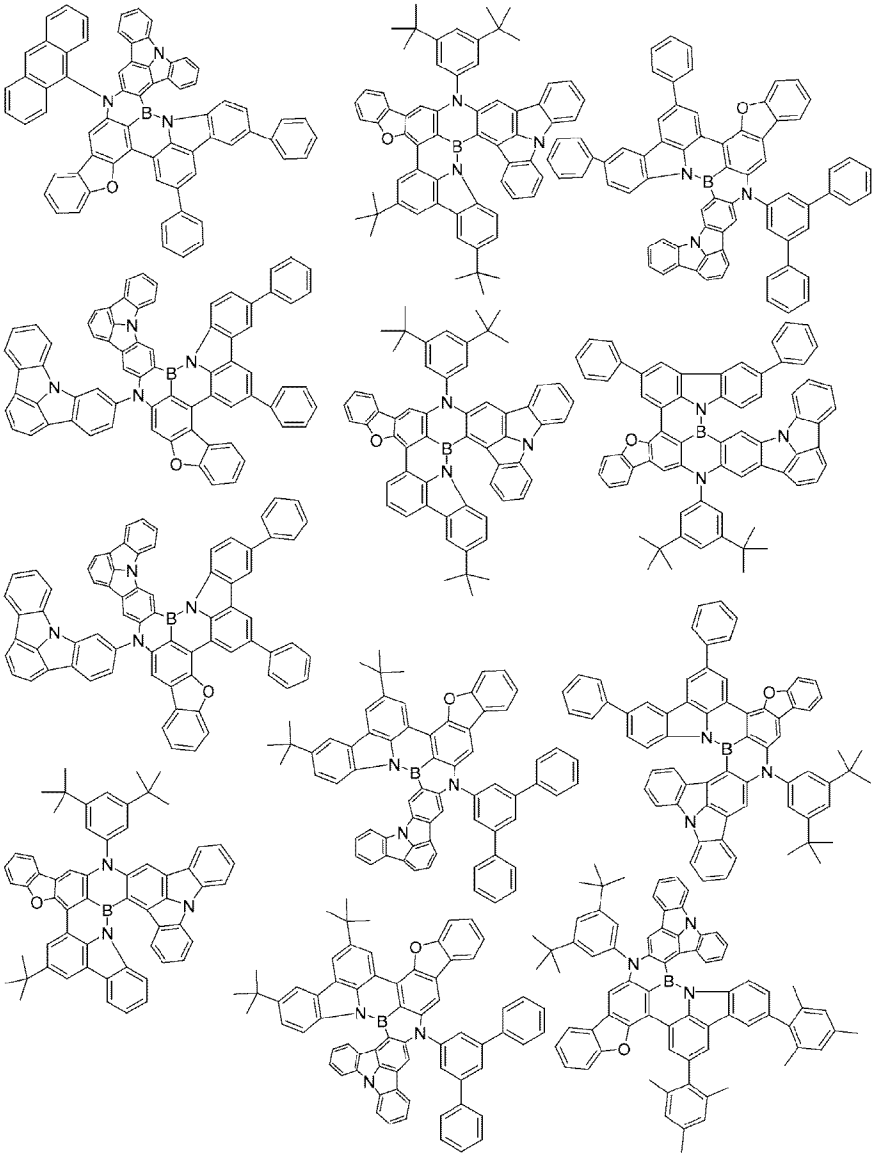
[774] OLED **D1** yielded an external quantum efficiency (EQE) at 1000 cd/m^2 of 20.4%. The emission maximum is at 532 nm with a FWHM of 28 nm at 5.2 V. The corresponding CIEx value is 0.32 and the CIEy value is 0.65.

[775] **Additional Examples of Organic Molecules of the Invention**

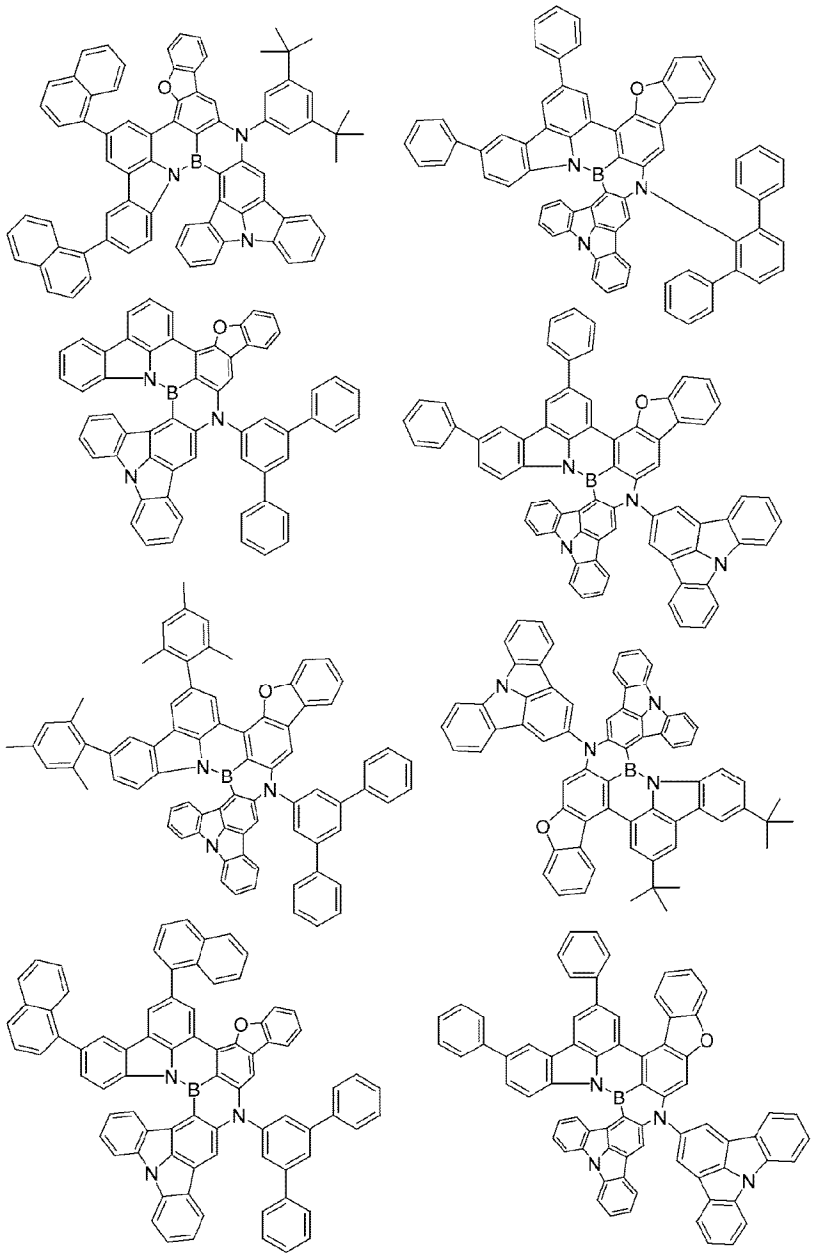
[776]



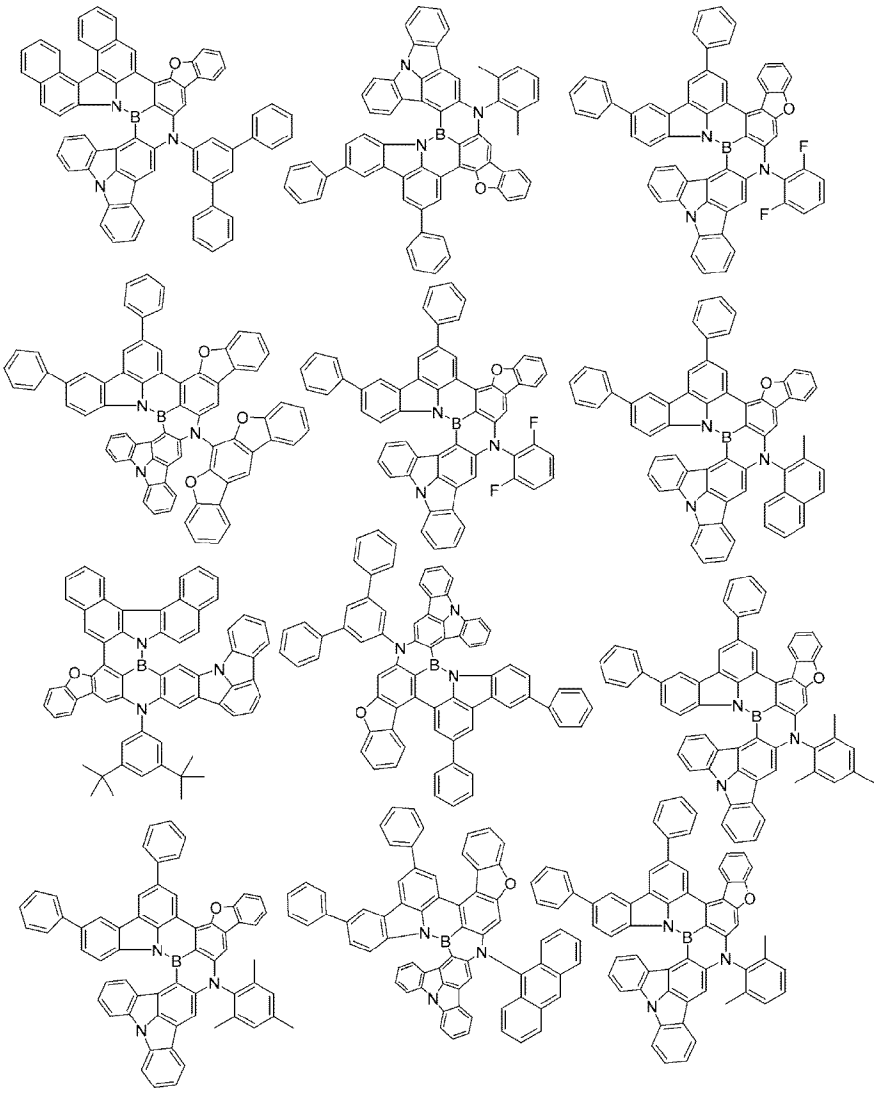
[777]



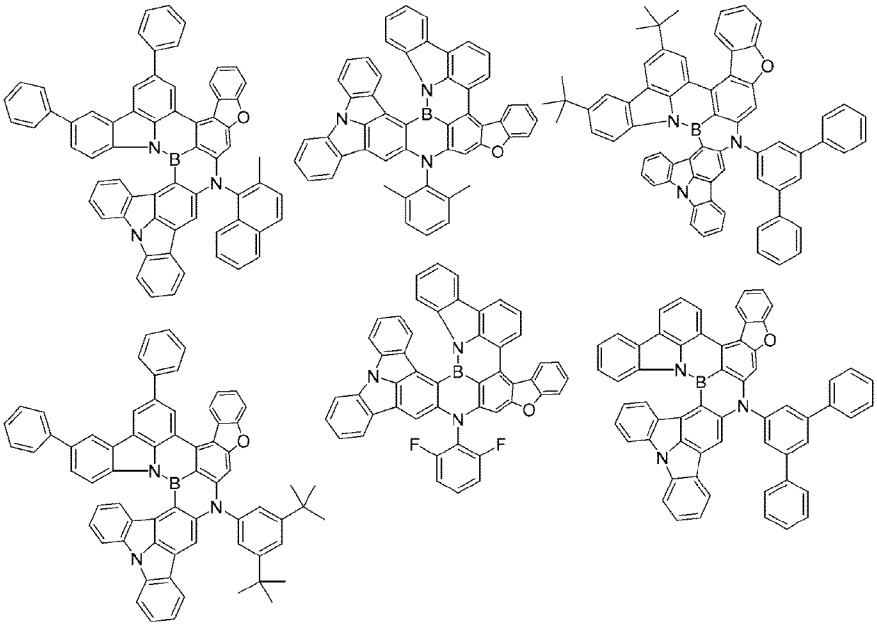
[778]



[779]

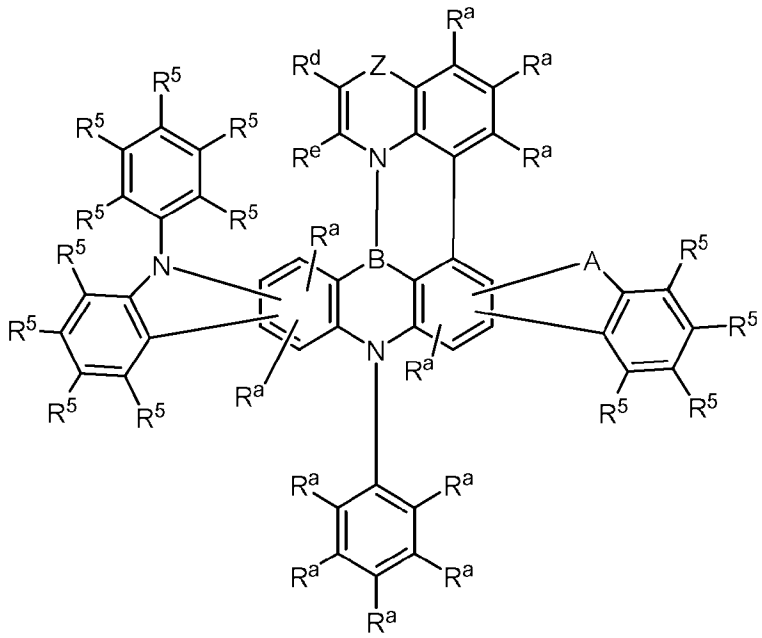


[780]



Claims

[Claim 1] Organic molecule, comprising a structure represented by formula I



Formula I

wherein

Z is at each occurrence independently selected from the group consisting of a direct bond, CR^3R^4, $C=CR^3R^4$, C=O, $C=NR^3$, NR^3, O, SiR^3R^4, S, S(O) and $S(O)_2$;

A is selected from the group consisting of O, S, and NR^5;

R^d and R^e is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^a)_2$, OR^a, $Si(R^a)_3$, $B(OR^a)_2$, $B(R^a)_2$, OSO_2R^a, CF_3, CN, F, Cl, Br, I,

C_1-C_{40}-alkyl,

which is optionally substituted with one or more substituents R^a and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

C_1-C_{40}-alkoxy,

which is optionally substituted with one or more substituents R^a and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

C_1-C_{40}-thioalkoxy,

which is optionally substituted with one or more substituents R^a and

wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

C_2-C_{40}-alkenyl,

which is optionally substituted with one or more substituents R^a and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

C_2-C_{40}-alkynyl,

which is optionally substituted with one or more substituents R^a and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^aC=CR^a$, C≡C, $Si(R^a)_2$, $Ge(R^a)_2$, $Sn(R^a)_2$, C=O, C=S, C=Se, $C=NR^a$, $P(=O)(R^a)$, SO, SO_2, NR^a, O, S or $CONR^a$;

C_6-C_{60}-aryl,

which is optionally substituted with one or more substituents R^a; and

C_2-C_{57}-heteroaryl,

which is optionally substituted with one or more substituents R^a;

R^a, R^3 and R^4 is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^5)_2$, OR^5, $Si(R^5)_3$, $B(OR^5)_2$, $B(R^5)_2$, OSO_2R^5, CF_3, CN, F, Cl, Br, I,

C_1-C_{40}-alkyl,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_1-C_{40}-alkoxy,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_1-C_{40}-thioalkoxy,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_2-C_{40}-alkenyl,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally sub-

stituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_2-C_{40}-alkynyl,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_6-C_{60}-aryl,

which is optionally substituted with one or more substituents R^5; and

C_2-C_{57}-heteroaryl,

which is optionally substituted with one or more substituents R^5;

R^5 is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, $N(R^6)_2$, OR^6, $Si(R^6)_3$, $B(OR^6)_2$, $B(R^6)_2$, OSO_2R^6, CF_3, CN, F, Br, I,

C_1-C_{40}-alkyl,

which is optionally substituted with one or more substituents R^6 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

C_1-C_{40}-alkoxy,

which is optionally substituted with one or more substituents R^6 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

C_1-C_{40}-thioalkoxy,

which is optionally substituted with one or more substituents R^6 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

C_2-C_{40}-alkenyl,

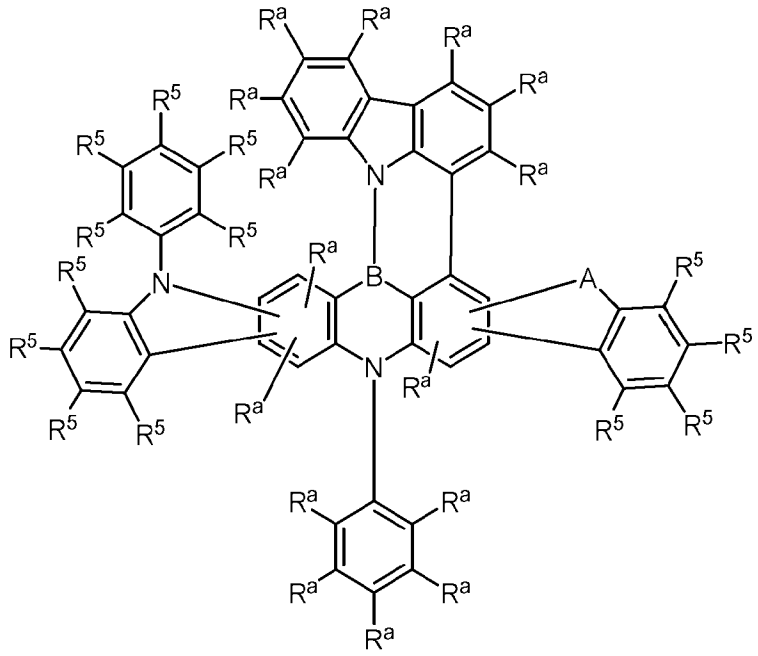
which is optionally substituted with one or more substituents R^6 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se, $C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;

C_2-C_{40}-alkynyl,

which is optionally substituted with one or more substituents R^6 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^6C=CR^6$, C≡C, $Si(R^6)_2$, $Ge(R^6)_2$, $Sn(R^6)_2$, C=O, C=S, C=Se,

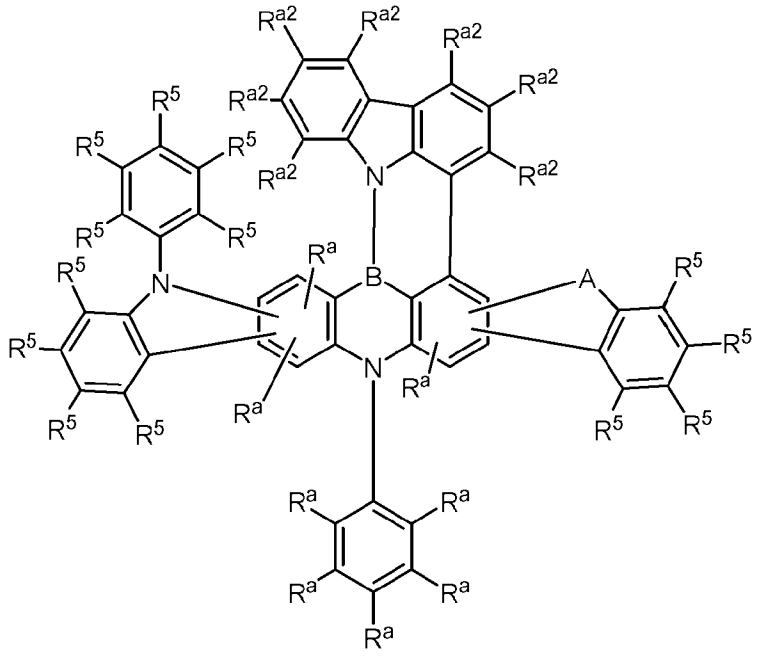
$C=NR^6$, $P(=O)(R^6)$, SO, SO_2, NR^6, O, S or $CONR^6$;
C_6-C_{60}-aryl,
which is optionally substituted with one or more substituents R^6; and
C_2-C_{57}-heteroaryl,
which is optionally substituted with one or more substituents R^6;
R^6 is at each occurrence independently selected from the group consisting of: hydrogen, deuterium, OPh, CF_3, CN, F,
C_1-C_5-alkyl,
wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;
C_1-C_5-alkoxy,
wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;
C_1-C_5-thioalkoxy,
wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;
C_2-C_5-alkenyl,
wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;
C_2-C_5-alkynyl,
wherein one or more hydrogen atoms are optionally, independently substituted by deuterium, CN, CF_3, or F;
C_6-C_{18}-aryl,
which is optionally substituted with one or more C_1-C_5-alkyl substituents;
C_2-C_{17}-heteroaryl,
which is optionally substituted with one or more C_1-C_5-alkyl substituents;
$N(C_6$-C_{18}-aryl$)_2$;
$N(C_2$-C_{17}-heteroaryl$)_2$, and
$N(C_2$-C_{17}-heteroaryl$)(C_6$-C_{18}-aryl);
wherein optionally, any of the substituents R^a, R^3, R^4, R^d, R^e, R^5, and R^6 independently form a mono- or polycyclic, aliphatic, aromatic, heteroaromatic and/or benzo-fused ring system with one or more substituents R^a, R^3, R^4, R^d, R^e, R^5 and/or R^6.

[Claim 2] The organic molecule according to claim 1, comprising a structure of formula Ia:



Formula Ia.

[Claim 3] The organic molecule according to claim 1 or 2, comprising a structure of formula Ia-2:



Formula Ia-2,

wherein R^{a2} is at each occurrence independently from another selected from the group consisting of:

hydrogen,

deuterium,

Me,

^{i}Pr,

^{t}Bu,

CN,

CF_3,

Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

pyridinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

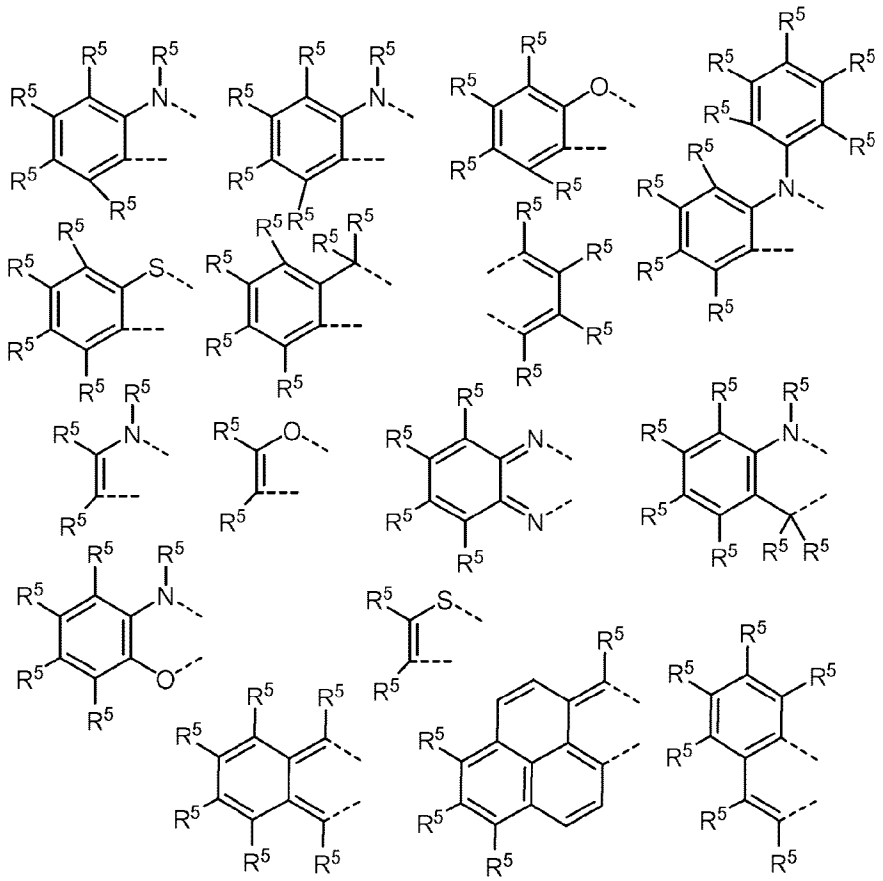
pyrimidinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

carbazolyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

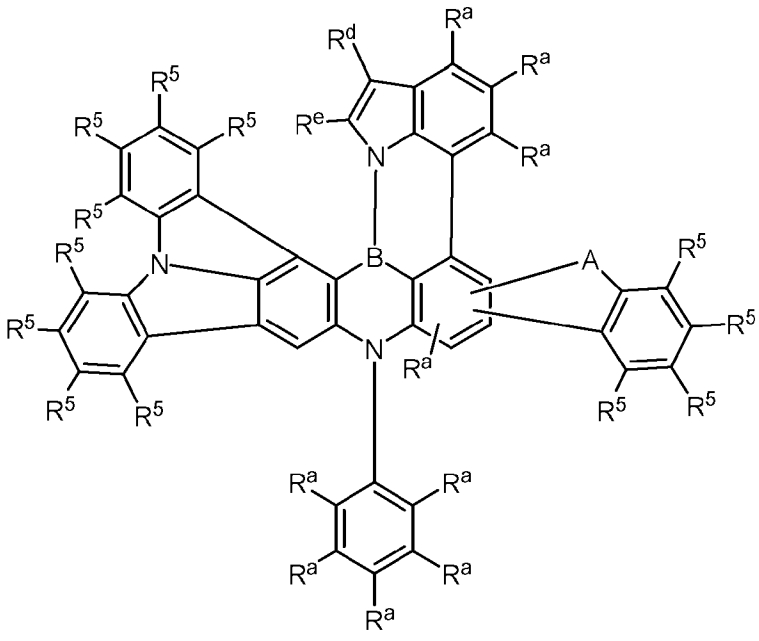
and $N(Ph)_2$, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph;

wherein two or more adjacent substituents R^a may form attachment points for a ring system selected from the group consisting of:

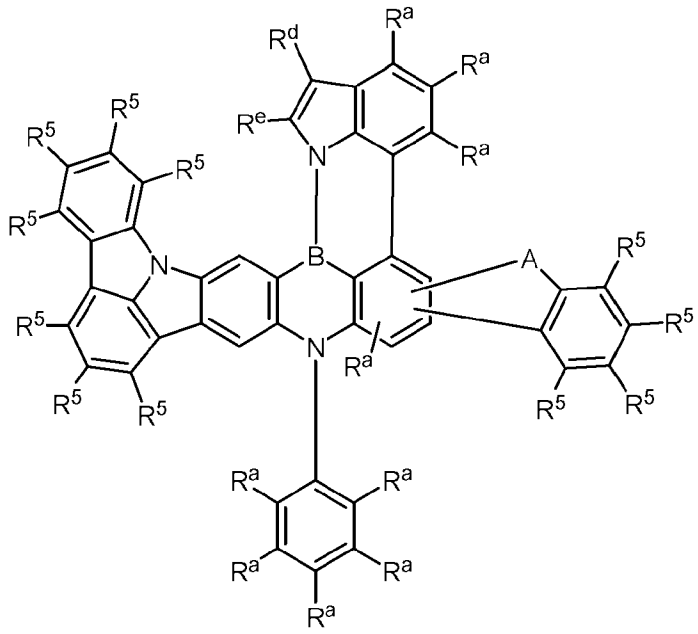


wherein each dashed line indicates a direct bond connecting one of the above shown ring systems to the positions of two adjacent substituents R^{a2} such that a ring system of the group shown above is fused to the structure as shown in Formula Ia-2.

[Claim 4] The organic molecule according to any of claims 1 to 3, comprising a structure of formula IIa or formula IIb:

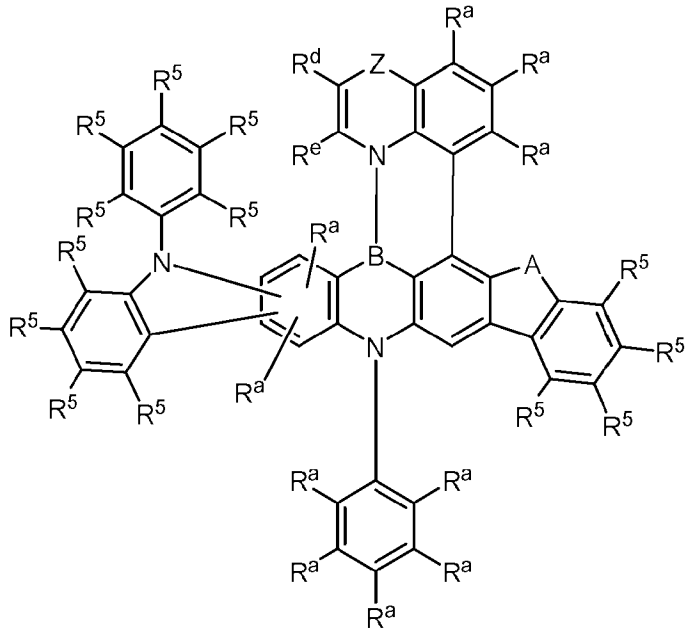


Formula IIa,

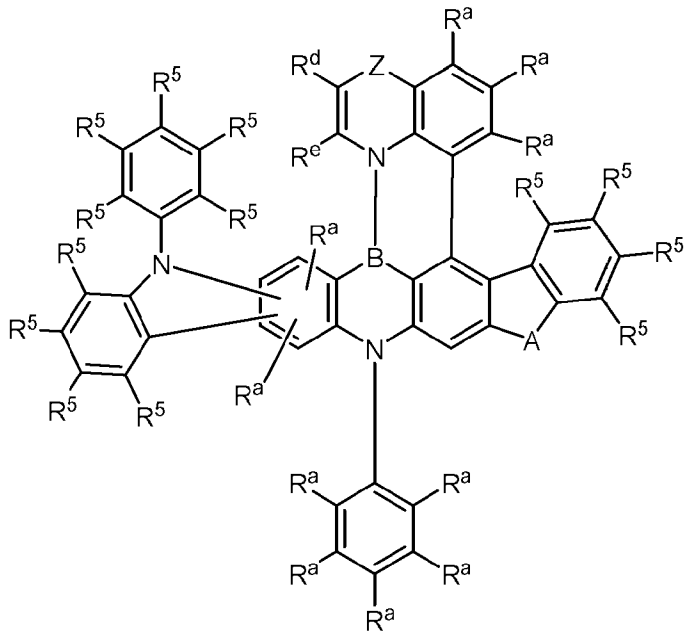


Formula IIb.

[Claim 5] The organic molecule according to any of claims 1 to 4, comprising a structure of formula IIIa or formula IIIb:

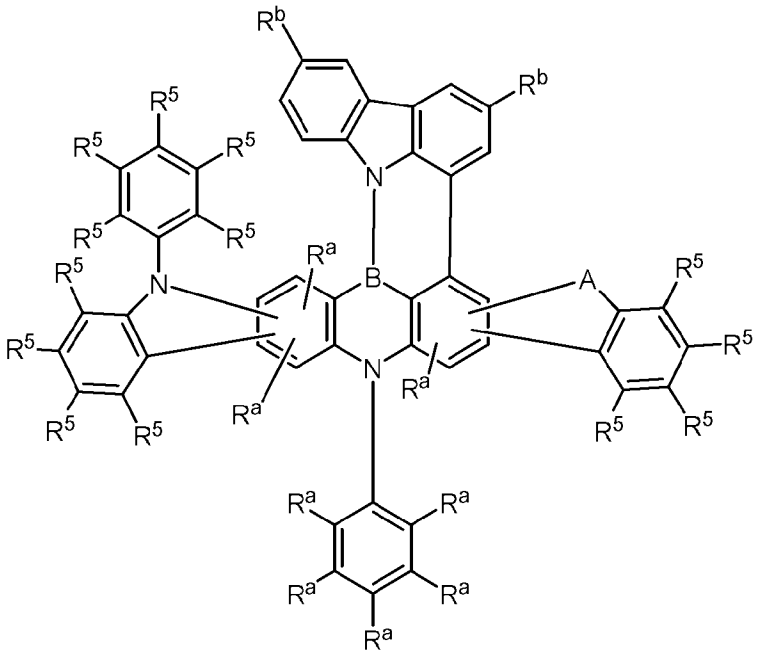


Formula IIIa,



Formula IIIb.

[Claim 6] The organic molecule according to any of claims 1 to 5, comprising a structure of formula Ib:



Formula Ib

wherein R^b is at each occurrence independently from another selected from the group consisting of hydrogen, deuterium, $N(R^5)_2$, OR^5, $Si(R^5)_3$, $B(OR^5)_2$, OSO_2R^5, CF_3, CN, F, Br, I,

C_1-C_{40}-alkyl,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally sub-

stituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_1-C_{40}-alkoxy,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_1-C_{40}-thioalkoxy,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_2-C_{40}-alkenyl,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

C_2-C_{40}-alkynyl,

which is optionally substituted with one or more substituents R^5 and wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C=CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C=NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;

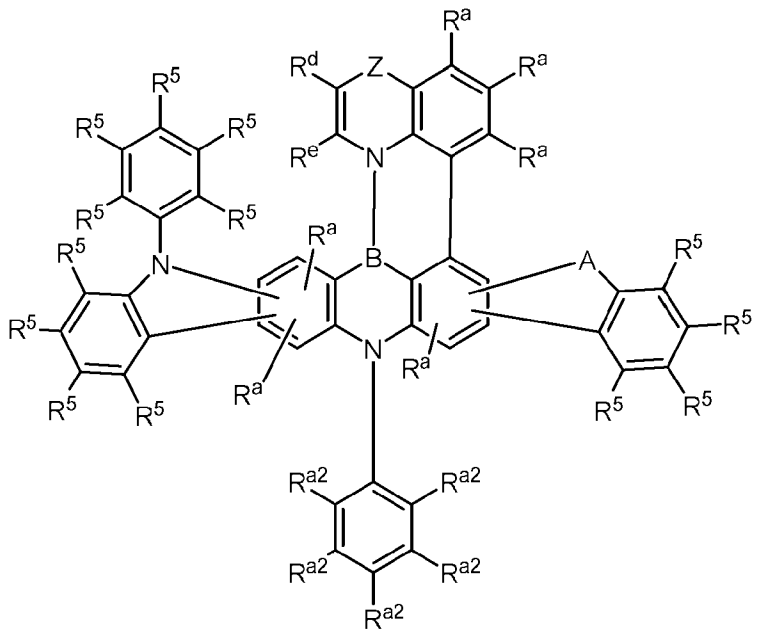
C_6-C_{60}-aryl,

which is optionally substituted with one or more substituents R^5; and

C_2-C_{57}-heteroaryl,

which is optionally substituted with one or more substituents R^5.

[Claim 7] The organic molecule according to any of claims 1 to 6, comprising a structure of formula IV:



Formula IV,

wherein R^{a2} is at each occurrence independently from another selected from the group consisting of:

hydrogen,

F,

Me,

^{i}Pr,

^{t}Bu,

Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

[Claim 8] Composition, comprising:

(a) an organic molecule according to any of claims 1 to 7, in particular in the form of an emitter, and

(b) a host material, which differs from the organic molecule, and

(c) optionally, a dye and/or a solvent.

[Claim 9] The composition according to claim 8 containing 0.1--30 % by weight, preferably 0.5--15 % by weight, in particular 0.7 - 5 % by weight, of the organic molecule.

[Claim 10] The composition according to claim 8 or 9, comprising a TADF material and/or a phosphorescence material.

[Claim 11] Optoelectronic device, comprising an organic molecule according to any of claims 1 to 7, in particular as a luminescent emitter, or a composition according to any of claims 8 to 10.

[Claim 12] The optoelectronic device according to claim 11, which is selected from the group consisting of:
· organic diodes,
· organic light-emitting diodes (OLEDs),
· light-emitting electrochemical cells,
· OLED-sensors,
· organic solar cells,
· organic transistors,
· organic field-effect transistors,
· organic lasers, and
· down-conversion elements.

[Claim 13] The optoelectronic device according to claim 11 or 12, comprising a phosphorescence material comprising iridium.

[Claim 14] The optoelectronic device according to any of claims 11 to 13, comprising:
- a substrate,
- an anode, and
- a cathode, wherein the anode or the cathode are disposed on the substrate, and
- a light-emitting layer, which is arranged between the anode and the cathode and which comprises the organic molecule or the composition.

[Claim 15] A method for generating light at a wavelength from 510 nm to 550 nm, comprising the steps of:
(i) providing an optoelectronic device according to any of claims 11 to 14; and
(ii) applying an electrical current to the optoelectronic device.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2022/020552

A. CLASSIFICATION OF SUBJECT MATTER

C07F 5/02(2006.01)i; **H10K 99/00**(2023.01)i; **H10K 50/00**(2023.01)i

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

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

C07F 5/02(2006.01); C09K 11/02(2006.01); C09K 11/06(2006.01); H01L 51/00(2006.01); H01L 51/50(2006.01)

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

Korean utility models and applications for utility models
Japanese utility models and applications for utility models

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

eKOMPASS(KIPO internal), STN(Registry, CAplus) & Keywords: OLED, organic light emitting diode, fused ring

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 2021-214306 A1 (CYNORA GMBH) 28 October 2021 (2021-10-28) abstract; pages 1-6, 19, 20, 55, 196	1-3
X	KR 10-2021-0084601 A (CYNORA GMBH) 07 July 2021 (2021-07-07) claim 1; page 44(1st compound, 10th compound)	1-3
X	CN 111471061 A (JIANGSU MARCH TECHNOLOGY CO., LTD.) 31 July 2020 (2020-07-31) claims 1, 2; page 4(compound (6))	1
A	US 2018-0114929 A1 (UNIVERSAL DISPLAY CORPORATION) 26 April 2018 (2018-04-26) the whole document	1-3
A	JP 2020-026426 A (KWANSEI GAKUIN UNIV et al.) 20 February 2020 (2020-02-20) the whole document	1-3

☐ Further documents are listed in the continuation of Box C. ☑ See patent family annex.

* Special categories of cited documents:
"A" document defining the general state of the art which is not considered to be of particular relevance
"D" document cited by the applicant in the international application
"E" earlier application or patent but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
20 March 2023	**21 March 2023**

Name and mailing address of the ISA/KR	Authorized officer
Korean Intellectual Property Office **189 Cheongsa-ro, Seo-gu, Daejeon** **35208, Republic of Korea**	**HEO, Joo Hyung**
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INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2022/020552

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☑ Claims Nos.: **9, 12**
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

Claims 9 and 12 are regarded to be unclear because they refer to claims which do not comply with PCT Rule 6.4(a).

3. ☑ Claims Nos.: **4-8, 10, 11, 13-15**
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

INTERNATIONAL SEARCH REPORT
Information on patent family members

International application No.
PCT/KR2022/020552

Patent document cited in search report	Publication date (day/month/year)	Patent family member(s)	Publication date (day/month/year)
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		EP 4139315 A1	01 March 2023
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CN 111471061 A	31 July 2020	None	
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JP 2020-026426 A	20 February 2020	None	