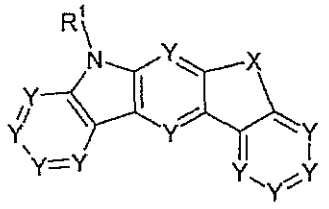
Patent Claims

1. Compound of the formula (1),



formula (1)

where the following applies to the symbols used:

Y is on each occurrence, identically or differently, CR or N;

X is selected from $C(R^1)_2$, O, S, PR^1, $P(=O)R^1$ or BR^1;

R, R^1 is on each occurrence, identically or differently, H, D, F, Cl, Br, I, $N(R^2)_2$, $N(Ar)_2$, $C(=O)Ar$, $P(=O)Ar_2$, $S(=O)Ar$, $S(=O)_2Ar$, $CR^2=CR^2Ar$, CN, NO_2, $Si(R^2)_3$, $B(OR^2)_2$, OSO_2R^2, a straight-chain alkyl, alkoxy or thioalkoxy group having 1 to 40 C atoms or a branched or cyclic alkyl, alkoxy or thioalkoxy group having 3 to 40 C atoms, each of which may be substituted by one or more radicals R^2, where one or more non-adjacent CH_2 groups may be replaced by $R^2C=CR^2$, C≡C, $Si(R^2)_2$, C=O, $C=NR^2$, $P(=O)(R^2)$, SO, SO_2, NR^2, O, S or $CONR^2$ and where one or more H atoms may be replaced by D, F, Cl, Br, I, CN or NO_2, or an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may in each case be substituted by one or more radicals R^2, or an aryloxy or heteroaryloxy group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^2, or an aralkyl or heteroaralkyl group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^2, or a combination of these systems; two or more substituents R here, together with the atoms to which they are bonded, or two substituents R^1, together with the atom to

which they are bonded, may also form a mono- or polycyclic, aliphatic or aromatic ring system with one another;

Ar is on each occurrence, identically or differently, an aromatic or heteroaromatic ring system having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^3;

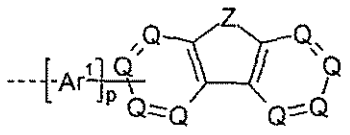
R^2 is on each occurrence, identically or differently, H, D, F, Cl, Br, I, $N(R^3)_2$, $N(Ar)_2$, C(=O)Ar, $P(=O)Ar_2$, S(=O)Ar, $S(=O)_2Ar$, $CR^3=CR^3Ar$, CN, NO_2, $Si(R^3)_3$, $B(OR^3)_2$, OSO_2R^3, a straight-chain alkyl, alkoxy or thioalkoxy group having 1 to 40 C atoms or a branched or cyclic alkyl, alkoxy or thioalkoxy group having 3 to 40 C atoms, each of which may be substituted by one or more radicals R^3, where one or more non-adjacent CH_2 groups may be replaced by $R^3C=CR^3$, C≡C, $Si(R^3)_2$, C=O, $C=NR^3$, $P(=O)(R^3)$, SO, SO_2, NR^3, O, S or $CONR^3$ and where one or more H atoms may be replaced by D, F, Cl, Br, I, CN or NO_2, or an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may in each case be substituted by one or more radicals R^3, or an aryloxy or heteroaryloxy group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^3, or an aralkyl or heteroaralkyl group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^3, or a combination of these systems;

R^3 is on each occurrence, identically or differently, H, D or an aliphatic hydrocarbon radical having 1 to 20 C atoms or an aryl or heteroaryl group having 5 to 40 ring atoms or a combination of these groups;

with the proviso that, if one or more of the groups R, R^1, R^2, R^3, Ar or Ar^1 contain heteroaryl groups which do not conform to the formulae (2), (3) or (4), these are not electron-deficient heteroaryl groups;

characterised in that at least one group R is present which stands, identically or differently on each occurrence, for a group of the follow-

ing formula (2),



formula (2)

where the dashed bond indicates the linking of the group of the formula (2), R^2 has the above-mentioned meanings, and furthermore:

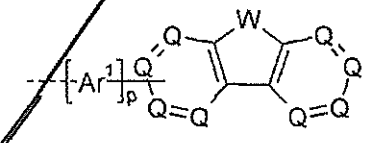
Q is C if the group of the formula (2) is linked to Ar^1 or to the remainder of the molecule via this group; or is, identically or differently on each occurrence, CR^2 or N in the other cases;

Z is NR^2 or S;

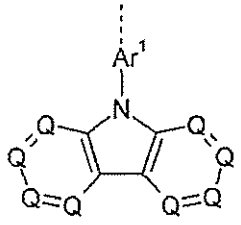
Ar^1 is a divalent aromatic or heteroaromatic ring system having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^2;

p is 0 or 1;

and/or in that at least one group R^1 is present which stands for a group of the following formula (3) or (4),



formula (3)



formula (4)

where the dashed bond indicates the linking of the group of the formula (3) or (4), R^2, Ar^1, Q and p have the above-mentioned meanings, and furthermore:

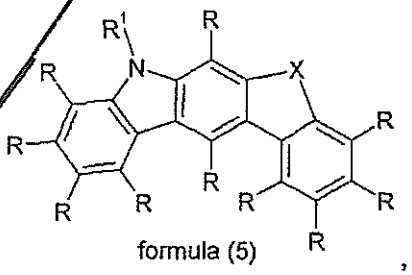
W is NR^2, O or S.

2. Compound according to Claim 1, characterised in that the radical R^1 which is bonded to the nitrogen atom stands for an aromatic or hetero-aromatic ring system having 5 to 60 aromatic ring atoms, which may also be substituted by one or more radicals R^2, or for a group of the formula (3) or (4).

3. Compound according to Claim 1 or 2, characterised in that X stands for $C(R^1)_2$, where R^1 stands, identically or differently on each occurrence, for a straight-chain alkyl group having 1 to 10 C atoms or a branched or cyclic alkyl group having 3 to 10 C atoms, each of which may be substituted by one or more radicals R^2, where one or more non-adjacent CH_2 groups may be replaced by $R^2C{=}CR^2$, $C{\equiv}C$, $Si(R^2)_2$, C=O, O, S or $CONR^2$ and where one or more H atoms may be replaced by D, F or CN, or for an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may also be substituted by one or more radicals R^2; the radicals R^1 here may also form an aromatic or aliphatic ring system with one another.

4. Compound according to one or more of Claims 1 to 3, characterised in that a maximum of one group Y per ring stands for N and the remaining groups Y stand, identically or differently on each occurrence, for CR.

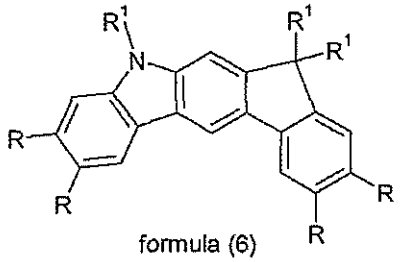
5. Compound according to one or more of Claims 1 to 4, selected from compounds of the formula (5),



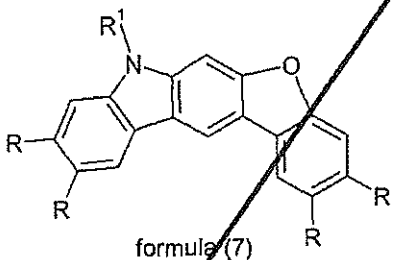
formula (5) ,

where the symbols used have the meanings given in Claim 1.

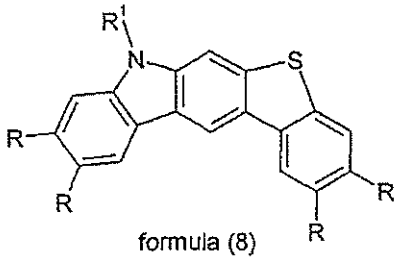
6. Compound according to Claim 5, selected from the structures of the formulae (6), (7) and (8),



formula (6)



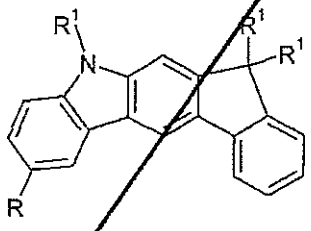
formula (7)



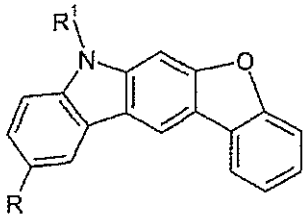
formula (8)

where the symbols used have the meanings given in Claim 1.

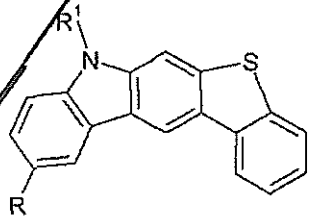
7. Compound according to Claim 6, selected from the compounds of the formulae (6b), (7b) and (8b),



formula (6b)



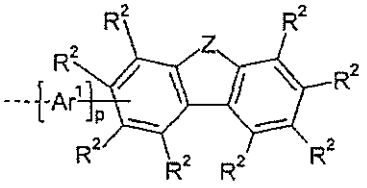
formula (7b)



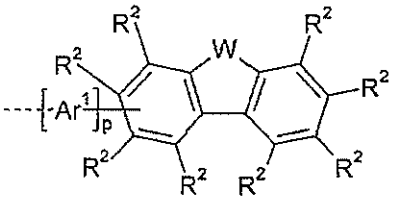
formula (8b)

where the symbols used have the meanings given in Claim 1.

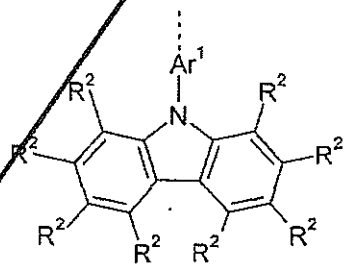
8. Compound according to one or more of Claims 1 to 7, characterised in that the groups of the formulae (2) to (4) are selected from the groups of the formulae (2a) to (4a),



formula (2a)



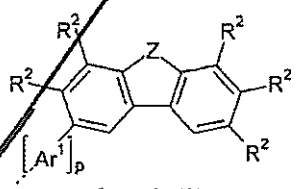
formula (3a)



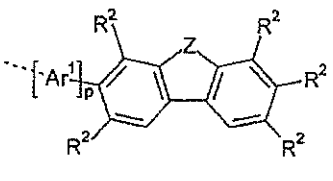
formula (4a)

where the symbols and indices used have the meanings given in Claim 1, and, in formula (2a) and (3a), no group R^2 is bonded at the position at which the group is linked to Ar^1 or the remainder of the molecule.

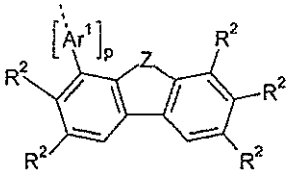
9. Compound according to one or more of Claims 1 to 8, characterised in that the groups of the formulae (2) to (4) are selected from the structures of the formulae (2b), (2c), (2d), (3b), (3c), (3d) and (4b),



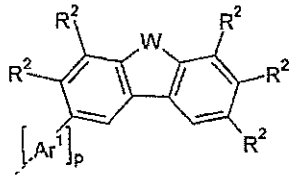
formula (2b)



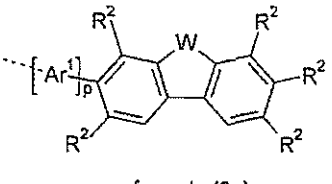
formula (2c)



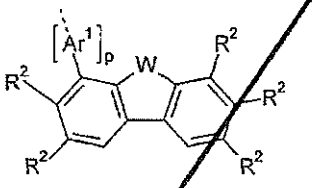
formula (2d)



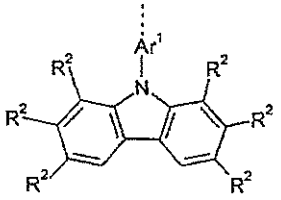
formula (3b)



formula (3c)



formula (3d)



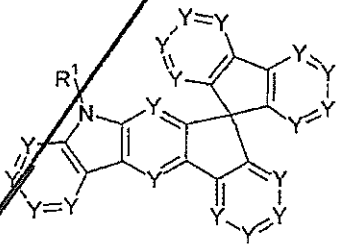
formula (4b)

where the dashed bond indicates the linking of the group to the remainder of the molecule, and the other symbols and indices used have the meanings given in Claim 1.

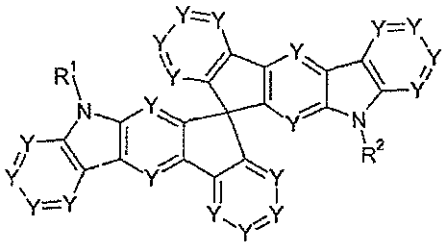
10. Compound according to Claim 8 or 9, characterised in that the radicals R^2 which are bonded to a carbon atom in formula (2a) to (4b) stand for H.

11. Compound according to one or more of Claims 1 to 10, characterised in that Z or W stands for NR^2, where R^2 stands for an aromatic or heteroaromatic ring system.

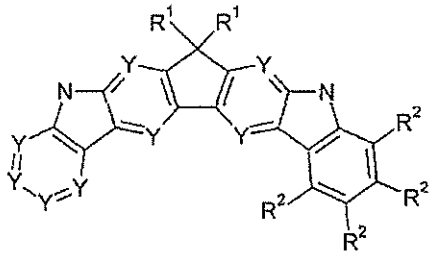
12. Compound according to one or more of Claims 1 to 11, selected from structures of the formula (9), (10), (11) or (12),



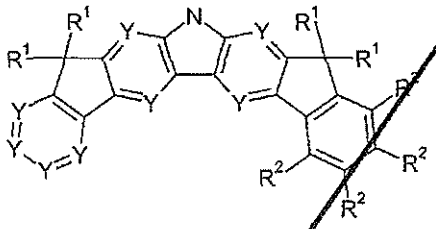
formula (9)



formula (10)



formula (11)



formula (12)

where the symbols used have the meanings given in Claim 1.

13. Process for the preparation of a compound according to one or more of Claims 1 to 12, characterised in that the group of the formula (2), (3) or (4) is introduced by a Suzuki coupling, an Ullmann coupling or by a Hartwig-Buchwald coupling.

14. Mixture comprising at least one compound according to one or more of Claims 1 to 12 and at least one fluorescent or phosphorescent dopant.

15. Formulation, in particular a solution, a suspension or a miniemulsion, comprising at least one compound according to one or more of Claims 1 to 12 or a mixture according to Claim 14 and one or more solvents.

16. Use of a compound according to one or more of Claims 1 to 12 or a mixture according to Claim 14 in an electronic device.

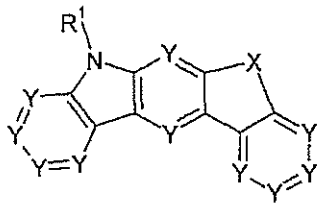
17. Electronic device, in particular selected from the group consisting of organic electroluminescent devices, organic integrated circuits, organic field-effect transistors, organic thin-film transistors, organic light-emitting transistors, organic solar cells, organic dye-sensitised solar cells, organic optical detectors, organic photoreceptors, organic field-quench devices, light-emitting electrochemical cells, organic laser diodes and "organic plasmon emitting devices", comprising at least one compound according to one or more of Claims 1 to 12 or a mixture according to Claim 14.

18. Electronic device according to Claim 17, characterised in that it is an organic electroluminescent device, and the compound according to

one or more of Claims 1 to 12 is employed as matrix material for a phosphorescent compound in an emitting layer.

Patent Claims

1. Compound of the formula (1),



formula (1)

where the following applies to the symbols used:

Y is on each occurrence, identically or differently, CR or N;

X is selected from $C(R^1)_2$, O, S, PR^1, $P(=O)R^1$ or BR^1;

R, R^1 is on each occurrence, identically or differently, H, D, F, Cl, Br, I, $N(R^2)_2$, $N(Ar)_2$, $C(=O)Ar$, $P(=O)Ar_2$, $S(=O)Ar$, $S(=O)_2Ar$, $CR^2=CR^2Ar$, CN, NO_2, $Si(R^2)_3$, $B(OR^2)_2$, OSO_2R^2, a straight-chain alkyl, alkoxy or thioalkoxy group having 1 to 40 C atoms or a branched or cyclic alkyl, alkoxy or thioalkoxy group having 3 to 40 C atoms, each of which may be substituted by one or more radicals R^2, where one or more non-adjacent CH_2 groups may be replaced by $R^2C=CR^2$, C≡C, $Si(R^2)_2$, C=O, $C=NR^2$, $P(=O)(R^2)$, SO, SO_2, NR^2, O, S or $CONR^2$ and where one or more H atoms may be replaced by D, F, Cl, Br, I, CN or NO_2, or an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may in each case be substituted by one or more radicals R^2, or an aryloxy or heteroaryloxy group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^2, or an aralkyl or heteroaralkyl group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^2, or a combination of these systems; two or more substituents R here, together with the atoms to which they are bonded, or two substituents R^1, together with the atom to

which they are bonded, may also form a mono- or polycyclic, aliphatic or aromatic ring system with one another;

Ar is on each occurrence, identically or differently, an aromatic or heteroaromatic ring system having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^3;

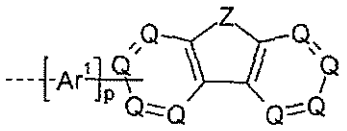
R^2 is on each occurrence, identically or differently, H, D, F, Cl, Br, I, $N(R^3)_2$, $N(Ar)_2$, $C(=O)Ar$, $P(=O)Ar_2$, $S(=O)Ar$, $S(=O)_2Ar$, $CR^3=CR^3Ar$, CN, NO_2, $Si(R^3)_3$, $B(OR^3)_2$, OSO_2R^3, a straight-chain alkyl, alkoxy or thioalkoxy group having 1 to 40 C atoms or a branched or cyclic alkyl, alkoxy or thioalkoxy group having 3 to 40 C atoms, each of which may be substituted by one or more radicals R^3, where one or more non-adjacent CH_2 groups may be replaced by $R^3C=CR^3$, C≡C, $Si(R^3)_2$, C=O, $C=NR^3$, $P(=O)(R^3)$, SO, SO_2, NR^3, O, S or $CONR^3$ and where one or more H atoms may be replaced by D, F, Cl, Br, I, CN or NO_2, or an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may in each case be substituted by one or more radicals R^3, or an aryloxy or heteroaryloxy group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^3, or an aralkyl or heteroaralkyl group having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^3, or a combination of these systems;

R^3 is on each occurrence, identically or differently, H, D or an aliphatic hydrocarbon radical having 1 to 20 C atoms or an aryl or heteroaryl group having 5 to 40 ring atoms or a combination of these groups;

with the proviso that, if one or more of the groups R, R^1, R^2, R^3, Ar or Ar^1 contain heteroaryl groups which do not conform to the formulae (2) or (3), these are not electron-deficient heteroaryl groups;

characterised in that at least one group R is present which stands, identically or differently on each occurrence, for a group of the follow-

ing formula (2),



formula (2)

where the dashed bond indicates the linking of the group of the formula (2), R^2 has the above-mentioned meanings, and furthermore:

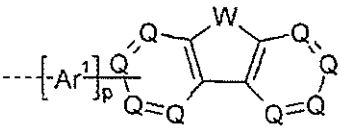
Q is C if the group of the formula (2) is linked to Ar^1 or to the remainder of the molecule via this group; or is, identically or differently on each occurrence, CR^2 or N in the other cases;

Z is NR^2 ;

Ar^1 is a divalent aromatic or heteroaromatic ring system having 5 to 40 aromatic ring atoms, which may be substituted by one or more radicals R^2;

p is 0 or 1;

and/or in that at least one group R^1 is present which stands for a group of the following formula (3),



formula (3)

where the dashed bond indicates the linking of the group of the formula (3), R^2, Ar^1, Q and p have the above-mentioned meanings, and furthermore:

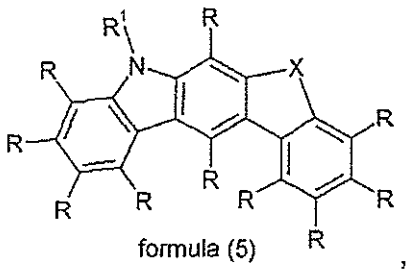
W is NR^2, O or S.

2. Compound according to Claim 1, characterised in that the radical R^1 which is bonded to the nitrogen atom stands for an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may also be substituted by one or more radicals R^2, or for a group of the formula (3).

3. Compound according to Claim 1 or 2, characterised in that X stands for $C(R^1)_2$, where R^1 stands, identically or differently on each occurrence, for a straight-chain alkyl group having 1 to 10 C atoms or a branched or cyclic alkyl group having 3 to 10 C atoms, each of which may be substituted by one or more radicals R^2, where one or more non-adjacent CH_2 groups may be replaced by $R^2C=CR^2$, C≡C, $Si(R^2)_2$, C=O, O, S or $CONR^2$ and where one or more H atoms may be replaced by D, F or CN, or for an aromatic or heteroaromatic ring system having 5 to 60 aromatic ring atoms, which may also be substituted by one or more radicals R^2; the radicals R^1 here may also form an aromatic or aliphatic ring system with one another.

4. Compound according to one or more of Claims 1 to 3, characterised in that a maximum of one group Y per ring stands for N and the remaining groups Y stand, identically or differently on each occurrence, for CR.

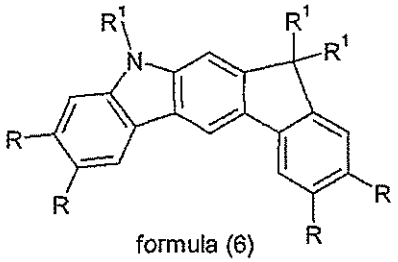
5. Compound according to one or more of Claims 1 to 4, selected from compounds of the formula (5),



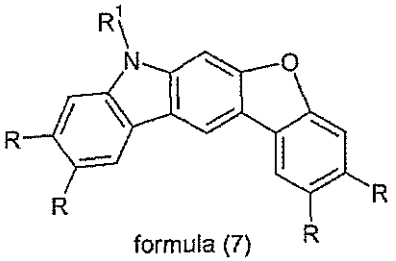
formula (5)

where the symbols used have the meanings given in Claim 1.

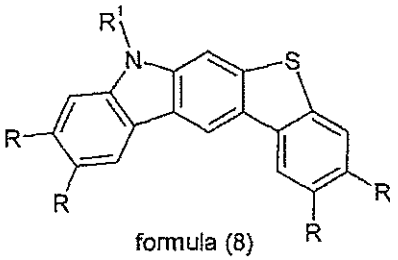
6. Compound according to Claim 5, selected from the structures of the formulae (6), (7) and (8),



formula (6)



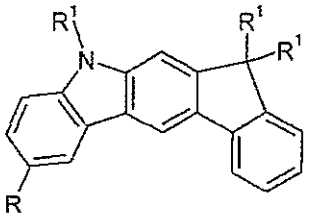
formula (7)



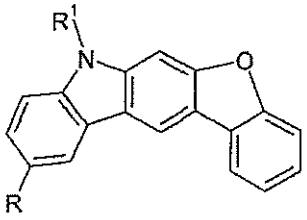
formula (8)

where the symbols used have the meanings given in Claim 1.

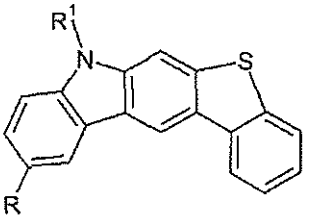
7. Compound according to Claim 6, selected from the compounds of the formulae (6b), (7b) and (8b),



formula (6b)



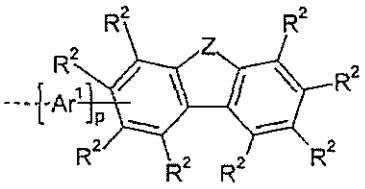
formula (7b)



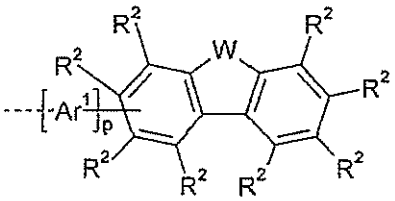
formula (8b)

where the symbols used have the meanings given in Claim 1.

8. Compound according to one or more of Claims 1 to 7, characterised in that the groups of the formulae (2) to (3) are selected from the groups of the formulae (2a) to (3a),



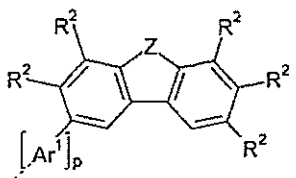
formula (2a)



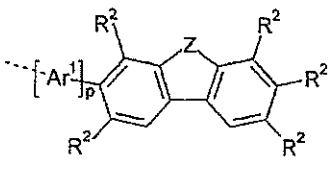
formula (3a)

where the symbols and indices used have the meanings given in Claim 1, and, in formula (2a) and (3a), no group R^2 is bonded at the position at which the group is linked to Ar^1 or the remainder of the molecule.

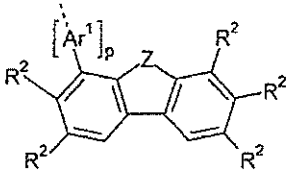
9. Compound according to one or more of Claims 1 to 8, characterised in that the groups of the formulae (2) to (3) are selected from the structures of the formulae (2b), (2c), (2d), (3b), (3c), and (3d),



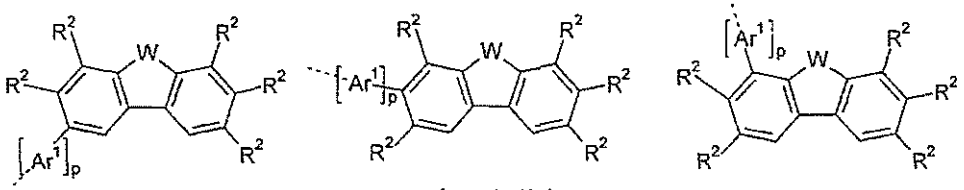
formula (2b)



formula (2c)



formula (2d)



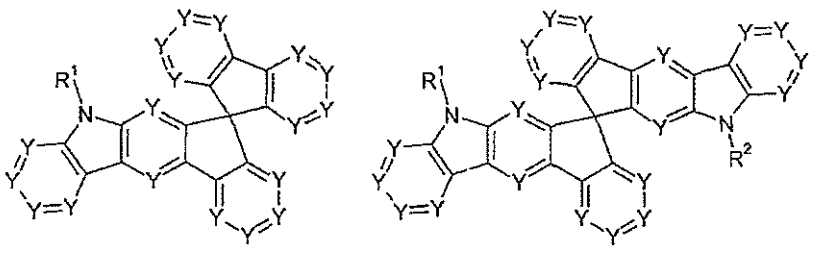
formula (3b) formula (3c) formula (3d)

where the dashed bond indicates the linking of the group to the remainder of the molecule, and the other symbols and indices used have the meanings given in Claim 1.

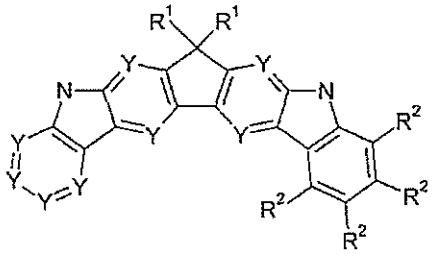
10. Compound according to Claim 8 or 9, characterised in that the radicals R^2 which are bonded to a carbon atom in formula (2a) to (3d) stand for H.

11. Compound according to one or more of Claims 1 to 10, characterised in that Z or W stands for NR^2, where R^2 stands for an aromatic or heteroaromatic ring system.

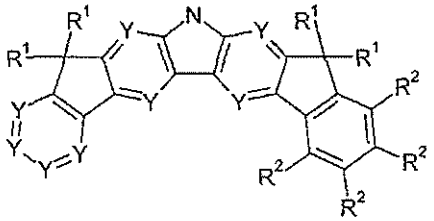
12. Compound according to one or more of Claims 1 to 11, selected from structures of the formula (9), (10), (11) or (12),



formula (9) formula (10)



formula (11)



formula (12)

where the symbols used have the meanings given in Claim 1.

13. Process for the preparation of a compound according to one or more of Claims 1 to 12, characterised in that the group of the formula (2). or (3) is introduced by a Suzuki coupling, an Ullmann coupling or by a Hartwig-Buchwald coupling.

14. Mixture comprising at least one compound according to one or more of Claims 1 to 12 and at least one fluorescent or phosphorescent dopant.

15. Formulation, in particular a solution, a suspension or a miniemulsion, comprising at least one compound according to one or more of Claims 1 to 12 or a mixture according to Claim 14 and one or more solvents.

16. Use of a compound according to one or more of Claims 1 to 12 or a mixture according to Claim 14 in an electronic device.

17. Electronic device, in particular selected from the group consisting of organic electroluminescent devices, organic integrated circuits, organic field-effect transistors, organic thin-film transistors, organic light-emitting transistors, organic solar cells, organic dye-sensitised solar cells, organic optical detectors, organic photoreceptors, organic field-quench devices, light-emitting electrochemical cells, organic laser diodes and "organic plasmon emitting devices", comprising at least one compound according to one or more of Claims 1 to 12 or a mixture according to Claim 14.

18. Electronic device according to Claim 17, characterised in that it is an organic electroluminescent device, and the compound according to

one or more of Claims 1 to 12 is employed as matrix material for a phosphorescent compound in an emitting layer.