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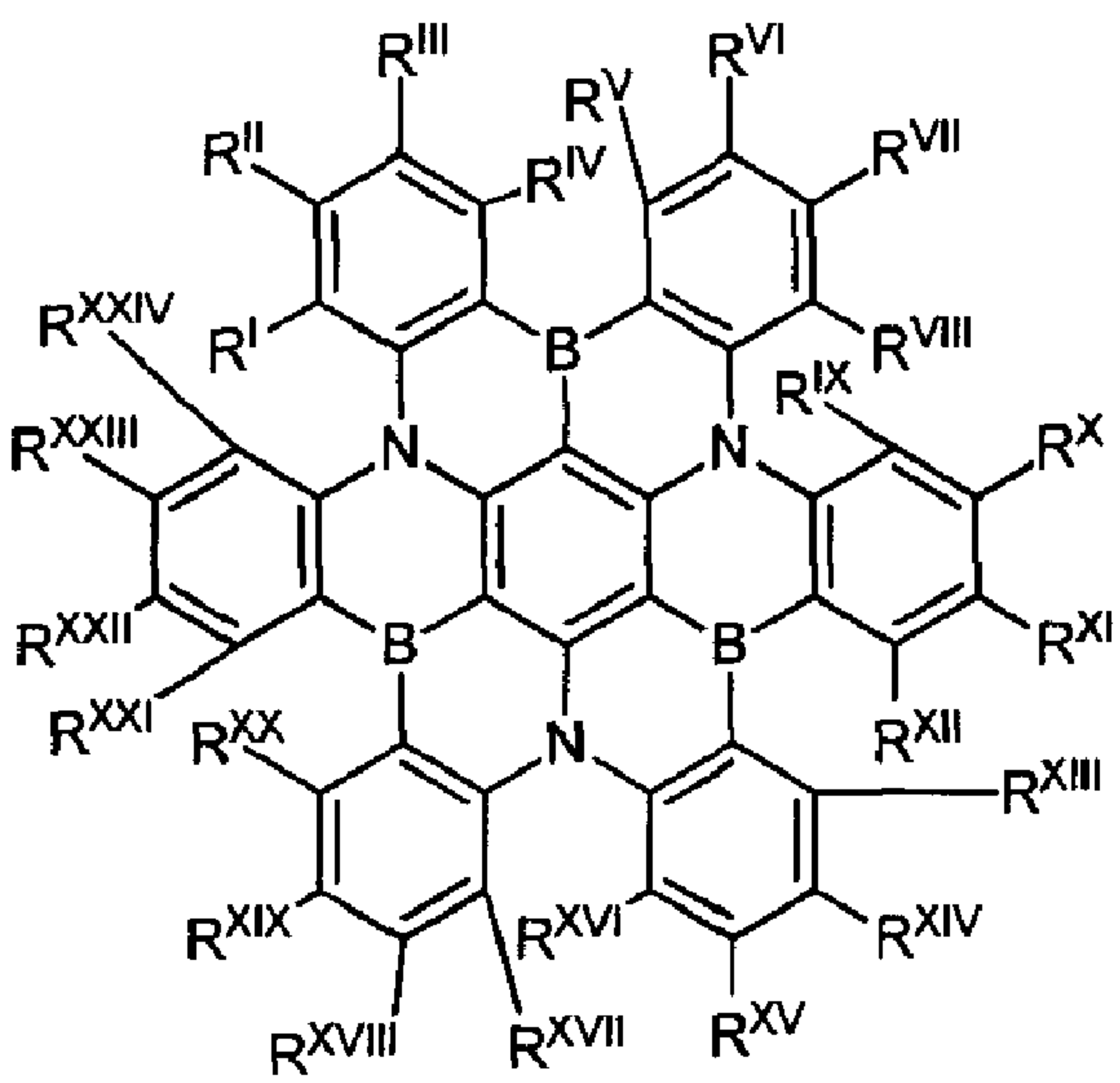
(54) Titre : MOLECULES ORGANIQUES, DESTINEES EN PARTICULIER AUX DISPOSITIFS OPTOELECTRONIQUES
(54) Title: ORGANIC MOLECULES, IN PARTICULAR FOR USE IN OPTOELECTRONIC DEVICES



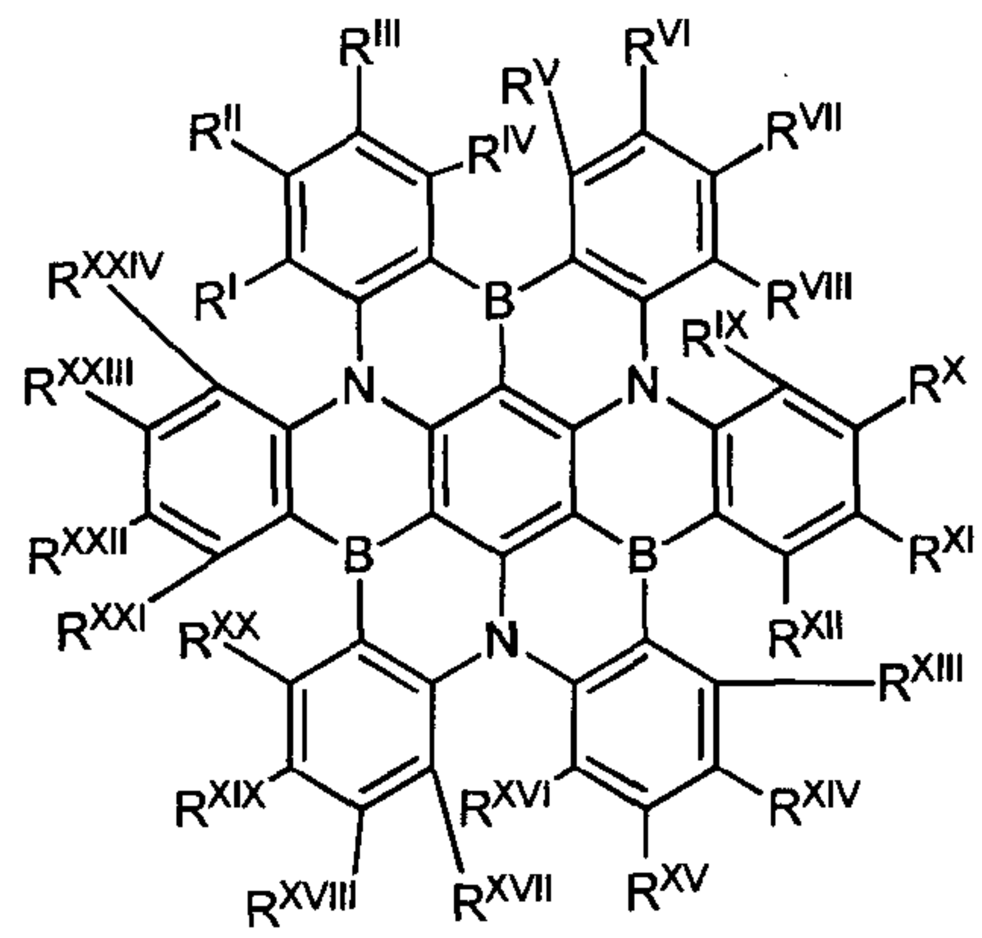
Formula I

(57) Abrégé/Abstract:
The invention relates to an organic compound, in particular for the use in optoelectronic devices. According to the invention, the organic compound has a structure of Formula I, <IMG> wherein R^{I}, R^{II}, R^{III}, R^{IV}, R^{V}, R^{VI}, R^{VII}, R^{VIII}, R^{X}, R^{XI}, R^{XII}, R^{XIII}, R^{XIV},

(57) **Abrégé(suite)/Abstract(continued):**
R^{XV}, R^{XVI}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} is independently from each other selected from the group consisting of: hydrogen, deuterium, C_1-C_{40}-alkoxyl, C_2-C_{40}-alkenyl, C_2-C_{40}-alkynyl, C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl, which is each optionally substituted with one or more substituents R^1; CN; CF_3; $N(R^1)_2$; OR^1, and $Si(R^1)_3$.

Abstract

The invention relates to an organic compound, in particular for the use in optoelectronic devices. According to the invention, the organic compound has a structure of Formula I,



Formula I

wherein

R^{I}, R^{II}, R^{III}, R^{IV}, R^{V}, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^{X}, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} is independently from each other selected from the group consisting of:

hydrogen, deuterium,

C_1-C_{40}-alkyl, C_1-C_{40}-alkoxyl,

C_2-C_{40}-alkenyl, C_2-C_{40}-alkynyl, C_6-C_{60}-aryl, C_3-C_{57}-heteroaryl,

which is each optionally substituted with one or more substituents R^1;

CN; CF_3; $N(R^1)_2$; OR^1, and $Si(R^1)_3$.

ORGANIC MOLECULES, IN PARTICULAR FOR USE IN OPTOELECTRONIC DEVICES

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

Description

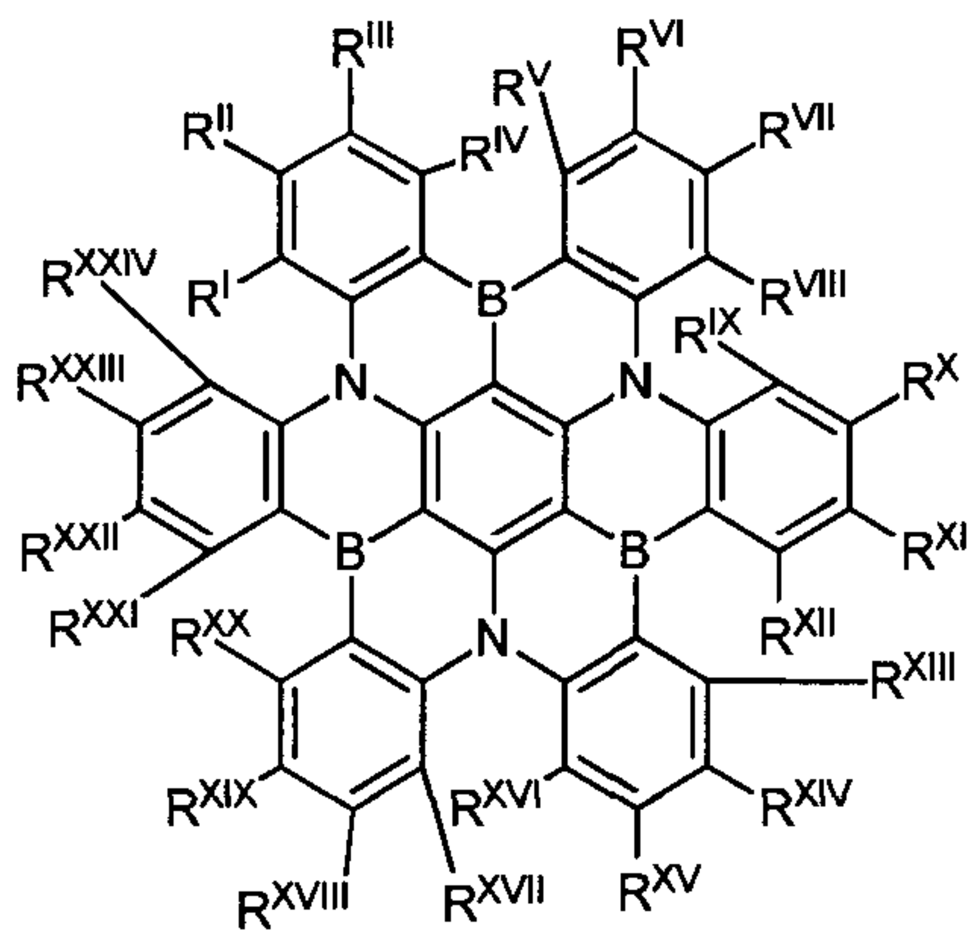
The object of the present invention is to provide molecules which are suitable for use in optoelectronic devices.

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

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.

According to the present invention, the organic molecules exhibit emission maxima in the blue, sky-blue or green spectral range. The organic molecules exhibit in particular emission maxima between 420 nm and 520 nm, preferably between 440 nm and 495 nm, more preferably between 450 nm and 470 nm. The photoluminescence quantum yields of the organic molecules according to the invention are, in particular, 20 % 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.

The organic light-emitting molecule of the invention comprises or consists of a structure of Formula I:



Formula I

wherein

R^{I}, R^{II}, R^{III}, R^{IV}, R^{V}, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^{X}, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} is independently from each other selected from the group consisting of:

hydrogen,

deuterium,

C_1-C_{40}-alkyl,

which is optionally substituted with one or more substituents R^1;

C_1-C_{40}-alkoxyl,

which is optionally substituted with one or more substituents R^1;

C_2-C_{40}-alkenyl,

which is optionally substituted with one or more substituents R^1;

C_2-C_{40}-alkynyl,

which is optionally substituted with one or more substituents R^1;

C_6-C_{60}-aryl,

which is optionally substituted with one or more substituents R^1;

C_3-C_{57}-heteroaryl,

which is optionally substituted with one or more substituents R^1;

CN;

CF_3;

$N(R^1)_2$;

OR^1, and

$Si(R^1)_3$.

R^1 is at each occurrence independently from another selected from the group consisting of: hydrogen, deuterium, OPh, CF_3, CN, F,

C_1-C_5-alkyl,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_1-C_5-alkoxy,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_1-C_5-thioalkoxy,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_2-C_5-alkenyl,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_2-C_5-alkynyl,

wherein optionally one or more hydrogen atoms are independently from each other 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_3-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_3-C_{17}-heteroaryl)$_2$; and

N(C_3-C_{17}-heteroaryl)(C_6-C_{18}-aryl).

Optionally at least one substituent selected from R^I, R^{II}, R^{III}, R^{IV}, R^V, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^X, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} independently from each other forms a mono- or polycyclic, aliphatic, aromatic and/or benzo-fused ring system with one or more substituents R^I, R^{II}, R^{III}, R^{IV}, R^V, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^X, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV}.

In a further embodiment of the invention, R^I, R^{II}, R^{III}, R^{IV}, R^V, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^X, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} is independently from another selected from the group consisting of:

hydrogen, deuterium, halogen, 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 $N(Ph)_2$.

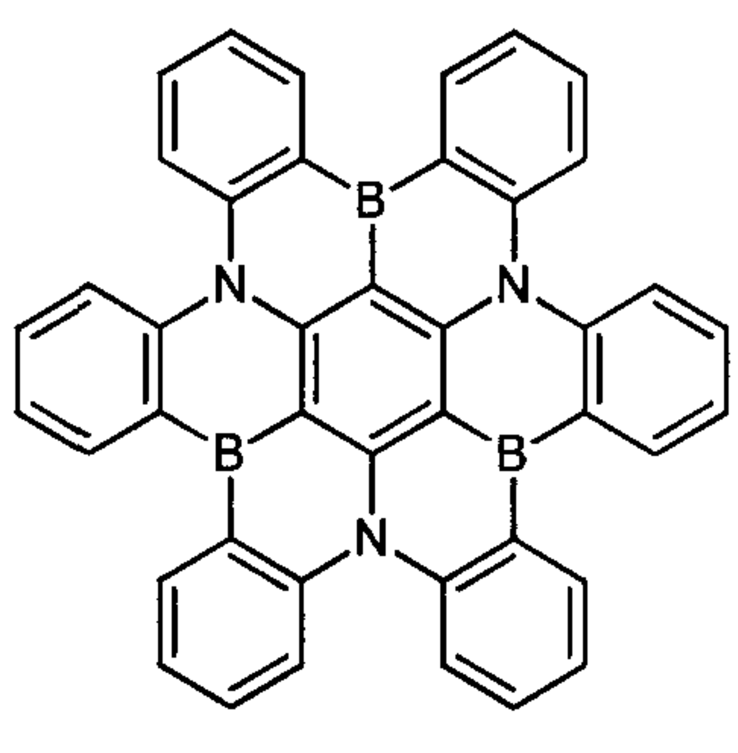
In a further embodiment of the invention, R^{II}, R^{IV}, R^{VI}, R^{VIII}, R^{X}, R^{XII}, R^{XIV}, R^{XVI}, R^{XVIII}, R^{XX}, R^{XXII} and R^{XXIV} is independently from another selected from the group consisting of:
hydrogen, deuterium, halogen, Me, ^{i}Pr, ^{t}Bu, CN, CF_3,
Ph, which is optionally 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, and
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 R^{I}, R^{III}, R^{V}, R^{VII}, R^{IX}, R^{XI}, R^{XIII}, R^{XV}, R^{XVII}, R^{XIX}, R^{XXI} and R^{XXIII} is independently from another selected from the group consisting of:
hydrogen, deuterium, 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, 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,
and $N(Ph)_2$.

In a further embodiment of the invention, R^{II}, R^{IV}, R^{VI}, R^{VIII}, R^{X}, R^{XII}, R^{XIV}, R^{XVI}, R^{XVIII}, R^{XX}, R^{XXII} and R^{XXIV} is independently from another selected from the group consisting of:
hydrogen, deuterium, Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and
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;
and R^{I}, R^{III}, R^{V}, R^{VII}, R^{IX}, R^{XI}, R^{XIII}, R^{XV}, R^{XVII}, R^{XIX}, R^{XXI} and R^{XXIII} is independently from another selected from the group consisting of hydrogen, deuterium, 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, and Ph,

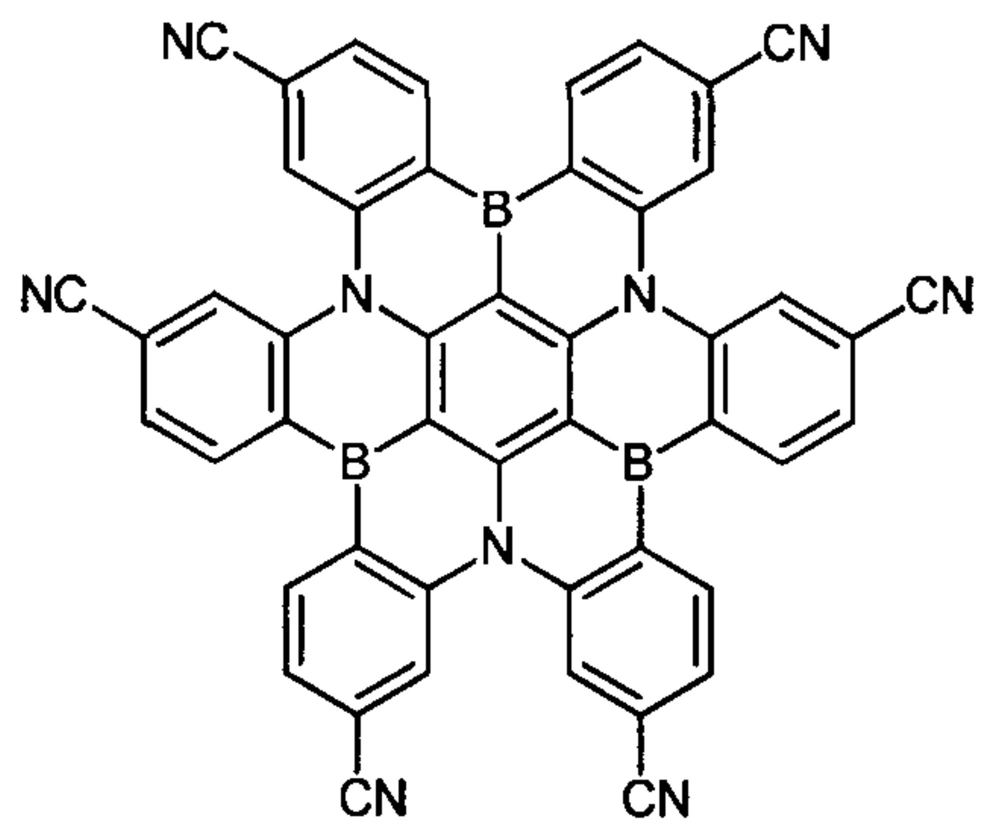
carbazolyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{t}Bu, and Ph
and $N(Ph)_2$.

In a further embodiment of the invention, R^{I}, R^{II}, R^{III}, R^{IV}, R^{V}, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^{X}, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} are each H.

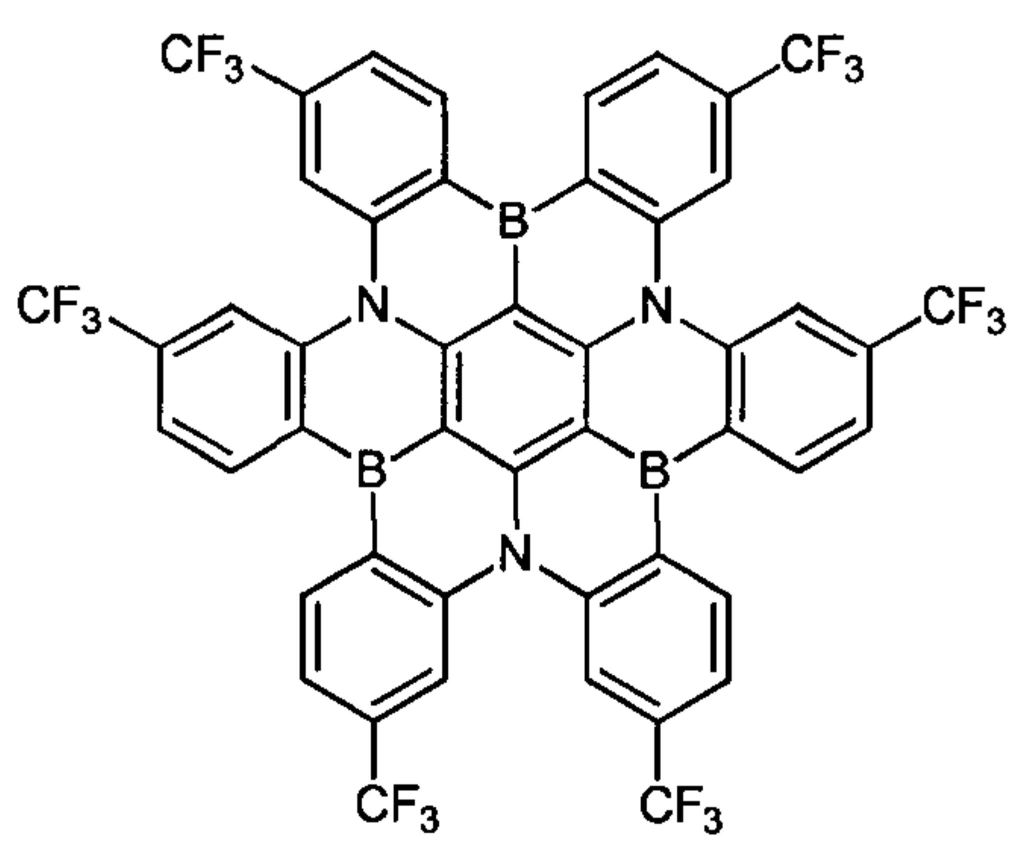
In a further embodiment of the invention, the organic molecules consist of a structure of one of Formulas II to IX:



Formula II



Formula III



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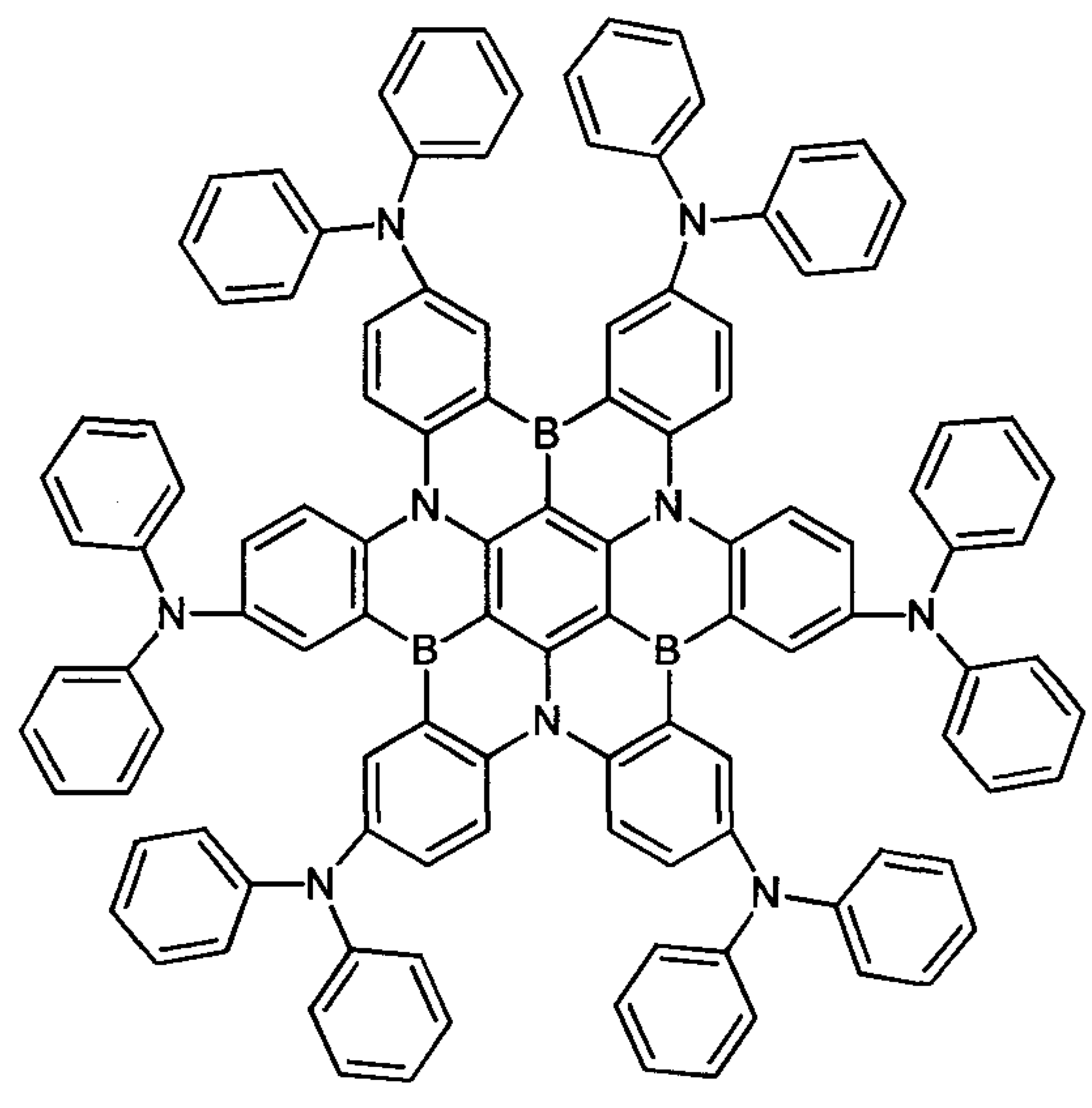
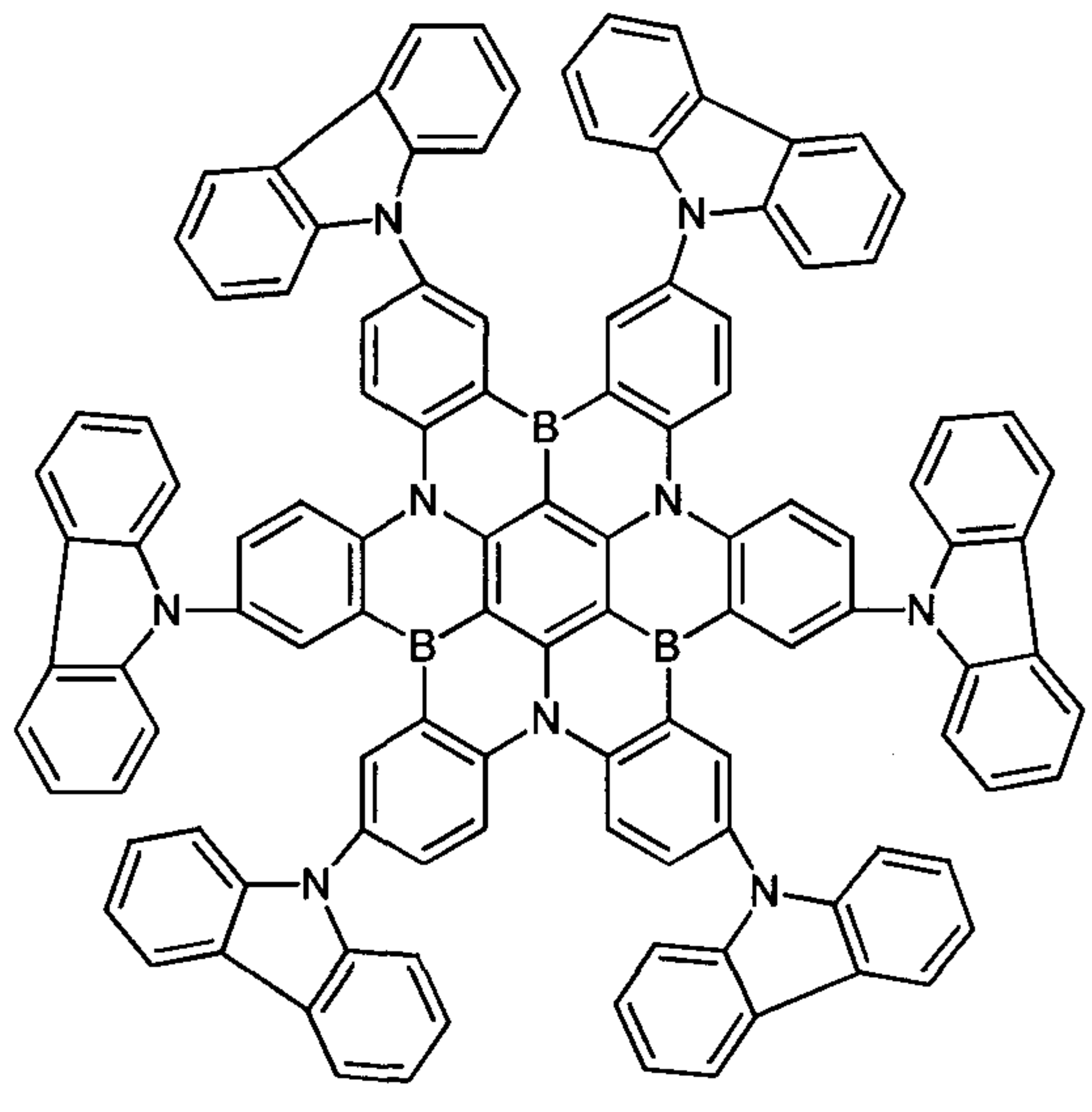
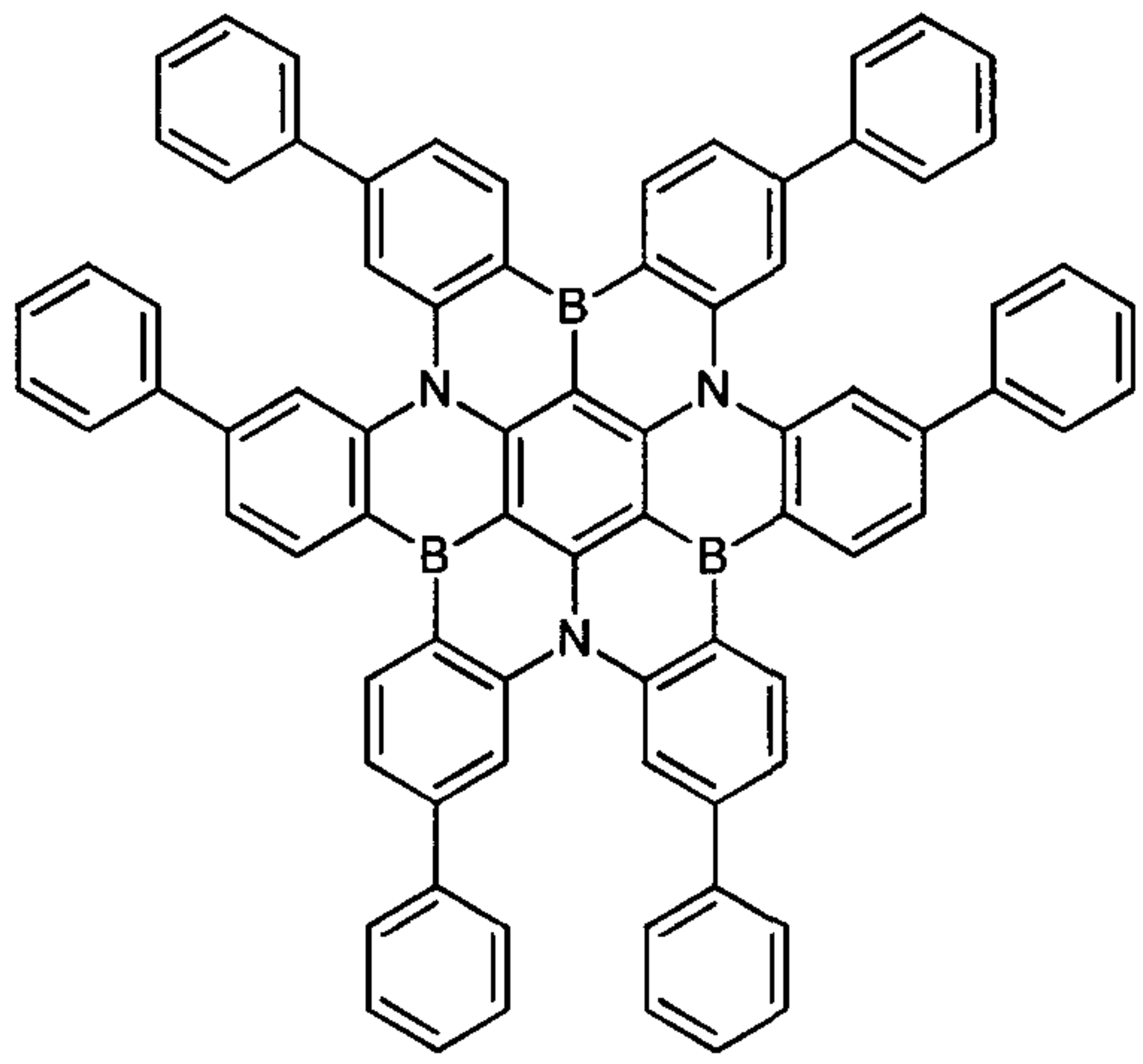


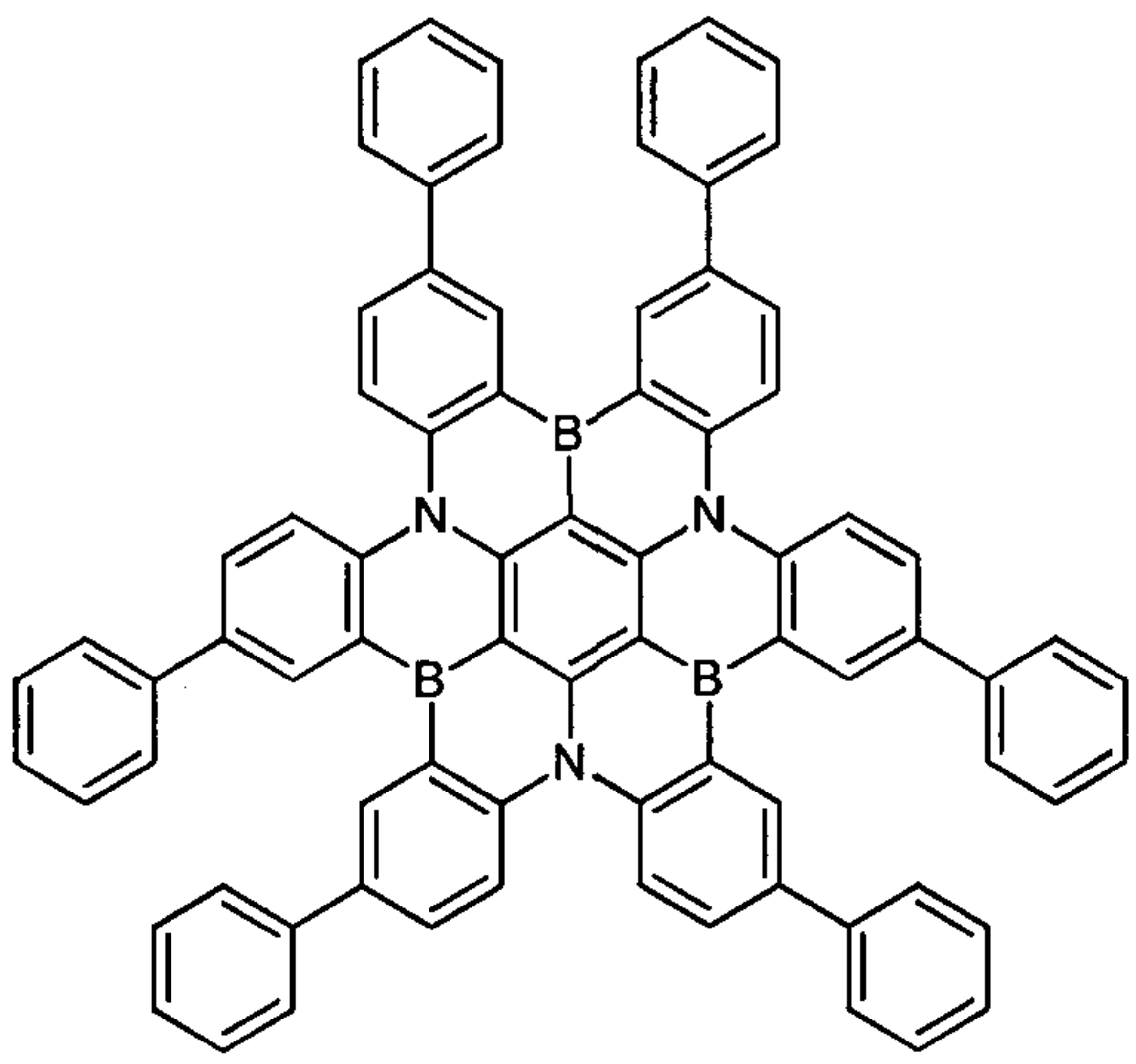
Formula VI



Formula VII



Formula VIII



Formula IX

As used throughout the present application, the terms "aryl" and "aromatic" may be understood in the broadest sense as any mono-, bi- or polycyclic aromatic moieties. Accordingly, an aryl group contains 6 to 60 aromatic ring atoms, and a heteroaryl group contains 5 to 60 aromatic ring atoms, of which at least one is a heteroatom. Notwithstanding, throughout the application the number of aromatic ring atoms may be given as subscripted number in the definition of certain substituents. In particular, the heteroaromatic ring includes one to three heteroatoms. Again, the terms “heteroaryl" and “heteroaromatic” may be understood in the broadest sense as any mono-, bi- or polycyclic hetero-aromatic moieties that include at least one heteroatom. The heteroatoms may at each occurrence be the same or different and be individually selected from the group consisting of N, O and S. Accordingly, the term "arylene" refers to a divalent substituent that bears two binding sites to other molecular structures and thereby serving as a linker structure. In case, a group in the exemplary embodiments is defined differently from the definitions given here, for example, the number of aromatic ring atoms or number of heteroatoms differs from the given definition, the definition in the exemplary embodiments is to be applied. According to the invention, a condensed (annulated) aromatic or heteroaromatic polycycle is built of two or more single aromatic or heteroaromatic cycles, which formed the polycycle via a condensation reaction.

In particular, as used throughout the present application, the term “aryl group or heteroaryl group” comprises groups which can be bound via any position of the aromatic or heteroaromatic group, derived from benzene, naphthaline, anthracene, phenanthrene, pyrene, dihydropyrene, chrysene, perylene, fluoranthene, benzanthracene, benzphenanthrene, tetracene, pentacene, benzpyrene, furan, benzofuran, isobenzofuran, dibenzofuran, thiophene, benzothiophene, isobenzothiophene, dibenzothiophene; pyrrole, indole, isoindole, carbazole, 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, 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, purine, pteridine, indolizine and benzothiadiazole or combinations of the abovementioned groups.

As used throughout the present application, the term “cyclic group” may be understood in the broadest sense as any mono-, bi- or polycyclic moieties.

As used throughout the present application, the term “biphenyl” as a substituent may be understood in the broadest sense as ortho-biphenyl, meta-biphenyl, or para-biphenyl, wherein ortho, meta and para is defined in regard to the binding site to another chemical moiety.

As used throughout the present application, the term “alkyl group” may be understood in the broadest sense as any linear, branched, or cyclic alkyl substituent. In particular, the term alkyl comprises the substituents 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, adamantyl, 2,2,2-trifluorethyl, 1,1-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.

As used throughout the present application, 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.

As used throughout the present application, the term “alkynyl” comprises linear, branched, and cyclic alkynyl substituents. The term alkynyl group exemplarily comprises ethynyl, propynyl, butynyl, pentynyl, hexynyl, heptynyl or octynyl.

As used throughout the present application, 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.

As used throughout the present application, the term “thioalkoxy” comprises linear, branched, and cyclic thioalkoxy substituents, in which the O of the exemplarily alkoxy groups is replaced by S.

As used throughout the present application, the terms “halogen” and “halo” may be understood in the broadest sense as being preferably fluorine, chlorine, bromine or iodine.

Whenever hydrogen (H) is mentioned herein, it could also be replaced by deuterium at each occurrence.

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 were a fragment (e.g. naphtyl, dibenzofuryl) or as if it were the whole molecule (e.g. naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

In one embodiment, the organic molecules according to the invention have an excited state lifetime of not more than 150 µs, of not more than 100 µs, in particular of not more than 50 µs, more preferably of not more than 10 µs or not more than 7 µs in a film of poly(methyl methacrylate) (PMMA) with 10 % by weight of organic molecule at room temperature.

In a further embodiment of the invention, the organic molecules according to the invention have an emission peak in the visible or nearest ultraviolet range, i.e., in the range of a wavelength of from 380 to 800 nm, with a full width at half maximum of less than 0.40 eV, preferably less than 0.35 eV, more preferably less than 0.33 eV, even more preferably less than 0.30 eV or even less than 0.28 eV in a film of poly(methyl methacrylate) (PMMA) with 10 % by weight of organic molecule at room temperature.

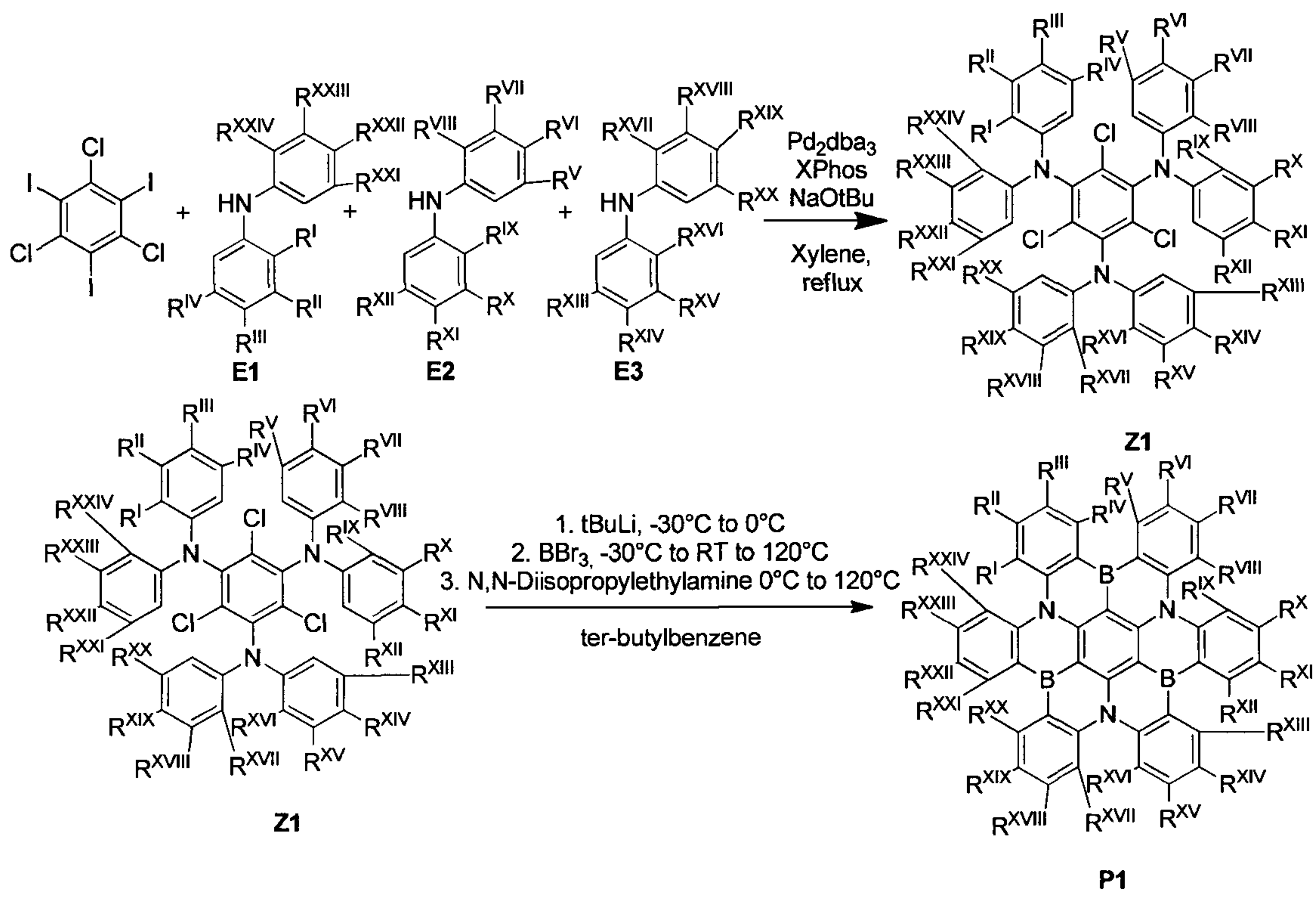
Orbital and excited state energies can be determined either by means of experimental methods or by calculations employing quantum-chemical methods, in particular density functional theory calculations. The energy of the highest occupied molecular orbital E^{HOMO} is determined by methods known to the person skilled in the art from cyclic voltammetry measurements with an accuracy of 0.1 eV. The energy of the lowest unoccupied molecular orbital E^{LUMO} is calculated as $E^{HOMO} + E^{gap}$, wherein E^{gap} is determined as follows: For host compounds, the onset of the emission spectrum of a film with 10 % by weight of host in poly(methyl methacrylate) (PMMA) is used as E^{gap}, unless stated otherwise. For emitter molecules, E^{gap} is determined as the energy at which the excitation and emission spectra of a film with 10 % by weight of emitter in PMMA cross.

The energy of the first excited triplet state T1 is determined from the onset of the emission spectrum at low temperature, typically at 77 K. For host compounds, where the first excited singlet state and the lowest triplet state are energetically separated by > 0.4 eV, the phosphorescence is usually visible in a steady-state spectrum in 2-Me-THF. The triplet energy can thus be determined as the onset of the phosphorescence spectrum. For TADF emitter molecules, the energy of the first excited triplet state T1 is determined from the onset of the delayed emission spectrum at 77

K, if not otherwise stated, measured in a film of PMMA with 10 % by weight of emitter. Both for host and emitter compounds, the energy of the first excited singlet state S1 is determined from the onset of the emission spectrum, if not otherwise stated, measured in a film of PMMA with 10 % by weight of host or emitter compound.

The onset of an emission spectrum is determined by computing the intersection of the tangent to the emission spectrum with the x-axis. The tangent to the emission spectrum is set at the high-energy side of the emission band and at the point at half maximum of the maximum intensity of the emission spectrum.

A further aspect of the invention relates to a process for preparing the organic molecule of the invention (with an optional subsequent reaction), wherein butyllithium (BuLi) and boron tribromide (BBr_3) are used as reactants:



A further aspect of the invention relates to the use of an organic molecule of the invention as a luminescent emitter or as an absorber, and/or as a host material and/or as an electron transport material, and/or as a hole injection material, and/or as a hole blocking material in an optoelectronic device.

A preferred embodiment relates to the use of an organic molecule according to the invention as a luminescent emitter in an optoelectronic device.

The optoelectronic device may be understood in the broadest sense as any device based on organic materials that is suitable for emitting light in the visible or nearest ultraviolet (UV) range, i.e., in the range of a wavelength of from 380 to 800 nm. More preferably, organic electroluminescent device may be able to emit light in the visible range, i.e., of from 400 nm to 800 nm.

In the context of such use, the optoelectronic device is more particularly selected from the group consisting of:

- organic light-emitting diodes (OLEDs),
- light-emitting electrochemical cells,
- OLED sensors, especially in gas and vapor sensors that are not hermetically shielded to the surroundings,
- organic diodes,
- organic solar cells,
- organic transistors,
- organic field-effect transistors,
- organic lasers and
- down-conversion elements.

In a preferred embodiment in the context of such use, the organic electroluminescent device is a device selected from the group consisting of an organic light emitting diode (OLED), a light emitting electrochemical cell (LEC), and a light-emitting transistor.

In the case of the use, the fraction of the organic molecule according to the invention in the emission layer in an optoelectronic device, more particularly in an OLED, is 1 % to 99 % by weight, more particularly 3 % to 80 % by weight. In an alternative embodiment, the proportion of the organic molecule in the emission layer is 100 % by weight.

In one embodiment, the light-emitting layer comprises not only the organic molecules according to the invention, but also a host material whose triplet (T1) and singlet (S1) energy levels are energetically higher than the triplet (T1) and singlet (S1) energy levels of the organic molecule.

A further aspect of the invention relates to a composition comprising or consisting of:

(a) at least one organic molecule according to the invention, in particular in the form of an emitter and/or a host, and

(b) one or more emitter and/or host materials, which differ from the organic molecule according to the invention and

(c) optional one or more dyes and/or one or more solvents.

In one embodiment, the light-emitting layer comprises (or essentially consists of) a composition comprising or consisting of:

(a) at least one organic molecule according to the invention, in particular in the form of an emitter and/or a host, and

(b) one or more emitter and/or host materials, which differ from the organic molecule according to the invention and

(c) optional one or more dyes and/or one or more solvents.

In a particular embodiment, the light-emitting layer EML comprises (or essentially consists of) a composition comprising or consisting of:

(i) 1-50 % by weight, preferably 5-40 % by weight, in particular 10-30 % by weight, of one or more organic molecules according to the invention;

(ii) 5-99 % by weight, preferably 30-94.9 % by weight, in particular 40-89% by weight, of at least one host compound H; and

(iii) optionally 0-94 % by weight, preferably 0.1-65 % by weight, in particular 1-50 % by weight, of at least one further host compound D with a structure differing from the structure of the molecules according to the invention; and

(iv) optionally 0-94 % by weight, preferably 0-65 % by weight, in particular 0-50 % by weight, of a solvent; and

(v) optionally 0-30 % by weight, in particular 0-20 % by weight, preferably 0-5 % by weight, of at least one further emitter molecule F with a structure differing from the structure of the molecules according to the invention.

Preferably, energy can be transferred from the host compound H to the one or more organic molecules according to the invention, in particular transferred from the first excited triplet state T1(H) of the host compound H to the first excited triplet state T1(E) of the one or more organic molecules according to the invention E and/ or from the first excited singlet state S1(H) of the host compound H to the first excited singlet state S1(E) of the one or more organic molecules according to the invention E.

In a further embodiment, the light-emitting layer EML comprises (or essentially consists of) a composition comprising or consisting of:

(i) 1-50 % by weight, preferably 5-40 % by weight, in particular 10-30 % by weight, of one organic molecule according to the invention;

(ii) 5-99 % by weight, preferably 30-94.9 % by weight, in particular 40-89% by weight, of one host compound H; and

(iii) optionally 0-94 % by weight, preferably 0.1-65 % by weight, in particular 1-50 % by weight, of at least one further host compound D with a structure differing from the structure of the molecules according to the invention; and

(iv) optionally 0-94 % by weight, preferably 0-65 % by weight, in particular 0-50 % by weight, of a solvent; and

(v) optionally 0-30 % by weight, in particular 0-20 % by weight, preferably 0-5 % by weight, of at least one further emitter molecule F with a structure differing from the structure of the molecules according to the invention.

In one embodiment, the host compound H has a highest occupied molecular orbital HOMO(H) having an energy $E^{HOMO}(H)$ in the range of from -5 to -6.5 eV and the at least one further host compound D has a highest occupied molecular orbital HOMO(D) having an energy $E^{HOMO}(D)$, wherein $E^{HOMO}(H) > E^{HOMO}(D)$.

In a further embodiment, the host compound H has a lowest unoccupied molecular orbital LUMO(H) having an energy $E^{LUMO}(H)$ and the at least one further host compound D has a lowest unoccupied molecular orbital LUMO(D) having an energy $E^{LUMO}(D)$, wherein $E^{LUMO}(H) > E^{LUMO}(D)$.

In one embodiment, the host compound H has a highest occupied molecular orbital HOMO(H) having an energy $E^{HOMO}(H)$ and a lowest unoccupied molecular orbital LUMO(H) having an energy $E^{LUMO}(H)$, and the at least one further host compound D has a highest occupied molecular orbital HOMO(D) having an energy $E^{HOMO}(D)$ and a lowest unoccupied molecular orbital LUMO(D) having an energy $E^{LUMO}(D)$,

the organic molecule according to the invention E has a highest occupied molecular orbital HOMO(E) having an energy $E^{HOMO}(E)$ and a lowest unoccupied molecular orbital LUMO(E) having an energy $E^{LUMO}(E)$,

wherein

$E^{HOMO}(H) > E^{HOMO}(D)$ and the difference between the energy level of the highest occupied molecular orbital HOMO(E) of the organic molecule according to the invention E ($E^{HOMO}(E)$) and the energy level of the highest occupied molecular orbital HOMO(H) of the host compound H ($E^{HOMO}(H)$) is between -0.5 eV and 0.5 eV, more preferably between -0.3 eV and 0.3 eV, even more preferably between -0.2 eV and 0.2 eV or even between -0.1 eV and 0.1 eV; and

$E^{LUMO}(H) > E^{LUMO}(D)$ and the difference between the energy level of the lowest unoccupied molecular orbital LUMO(E) of the organic molecule according to the invention E ($E^{LUMO}(E)$) and the lowest unoccupied molecular orbital LUMO(D) of the at least one further host compound D ($E^{LUMO}(D)$) is between -0.5 eV and 0.5 eV, more preferably between -0.3 eV and 0.3 eV, even more preferably between -0.2 eV and 0.2 eV or even between -0.1 eV and 0.1 eV.

In one embodiment of the invention the host compound D and/ or the host compound H is a thermally-activated delayed fluorescence (TADF)-material. TADF materials exhibit a ΔE_{ST} value, which corresponds to the energy difference between the first excited singlet state (S1) and the first excited triplet state (T1), of less than 2500 cm^{-1}. Preferably the TADF material exhibits a ΔE_{ST} value of less than 3000 cm^{-1}, more preferably less than 1500 cm^{-1}, even more preferably less than 1000 cm^{-1} or even less than 500 cm^{-1}.

In one embodiment, the host compound D is a TADF material and the host compound H exhibits a ΔE_{ST} value of more than 2500 cm^{-1}. In a particular embodiment, the host compound D is a TADF material and the host compound H is selected from group consisting of 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.

In one embodiment, the host compound H is a TADF material and the host compound D exhibits a ΔE_{ST} value of more than 2500 cm^{-1}. In a particular embodiment, the host compound H is a TADF material and the host compound D is selected from group consisting of 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).

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.

In a preferred embodiment, the organic electroluminescent device is a device selected from the group consisting of an organic light emitting diode (OLED), a light emitting electrochemical cell (LEC), and a light-emitting transistor.

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.

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.

When the organic electroluminescent device is an OLED, it may, for example, have the following layer structure:

1. substrate
2. anode layer A
3. hole injection layer, HIL
4. hole transport layer, HTL
5. electron blocking layer, EBL
6. emitting layer, EML
7. hole blocking layer, HBL
8. electron transport layer, ETL
9. electron injection layer, EIL
10. cathode layer,

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.

Furthermore, the organic electroluminescent 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.

In one embodiment of the invention, the organic electroluminescent device is an OLED, with the following inverted layer structure:

1. substrate
2. cathode layer
3. electron injection layer, EIL
4. electron transport layer, ETL
5. hole blocking layer, HBL
6. emitting layer, B
7. electron blocking layer, EBL
8. hole transport layer, HTL
9. hole injection layer, HIL
10. anode layer A

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.

In one embodiment of the invention, the organic electroluminescent 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.

In one embodiment of the invention, the organic electroluminescent 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.

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 polythiophene.

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 exemplarily 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).

Adjacent to the anode layer A or 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 such as vanadium oxide, molybdenum oxide or tungsten oxide may exemplarily be used as inorganic dopant. Tetrafluorotetracyanoquinodimethane (F_4-TCNQ), copper-pentafluorobenzoate (Cu(I)pFBz) or transition metal complexes may exemplarily be used as organic dopant.

The EBL may exemplarily 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).

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. Exemplarily, 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.

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.

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 such as Liq. The electron transport layer (ETL) may also block holes or a holeblocking layer (HBL) is introduced.
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).

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.

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.

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

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).

Optionally, an organic electroluminescent device (e.g., an OLED) may, for example, be an essentially white organic electroluminescent device. Exemplarily such white organic electroluminescent 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.

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:

violet:	wavelength range of >380-420 nm;
deep blue:	wavelength range of >420-480 nm;
sky blue:	wavelength range of >480-500 nm;
green:	wavelength range of >500-560 nm;
yellow:	wavelength range of >560-580 nm;
orange:	wavelength range of >580-620 nm;
red:	wavelength range of >620-800 nm.

With respect to emitter molecules, such colors refer to the emission maximum. Therefore, exemplarily, 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.

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.

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.

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 0.40 eV, preferably less than 0.35 eV, more preferably less than 0.33 eV, even more preferably less than 0.30 eV or even less than 0.28 eV.

A further aspect of the present invention relates to an OLED, which emits light with CIEx and CIEy color coordinates close to the CIEx (= 0.131) and CIEy (= 0.046) color coordinates of the primary color blue (CIEx = 0.131 and CIEy = 0.046) 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. Accordingly, a further aspect of the present invention relates to an OLED, 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.

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.

The organic electroluminescent 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

- prepared by means of a sublimation process,

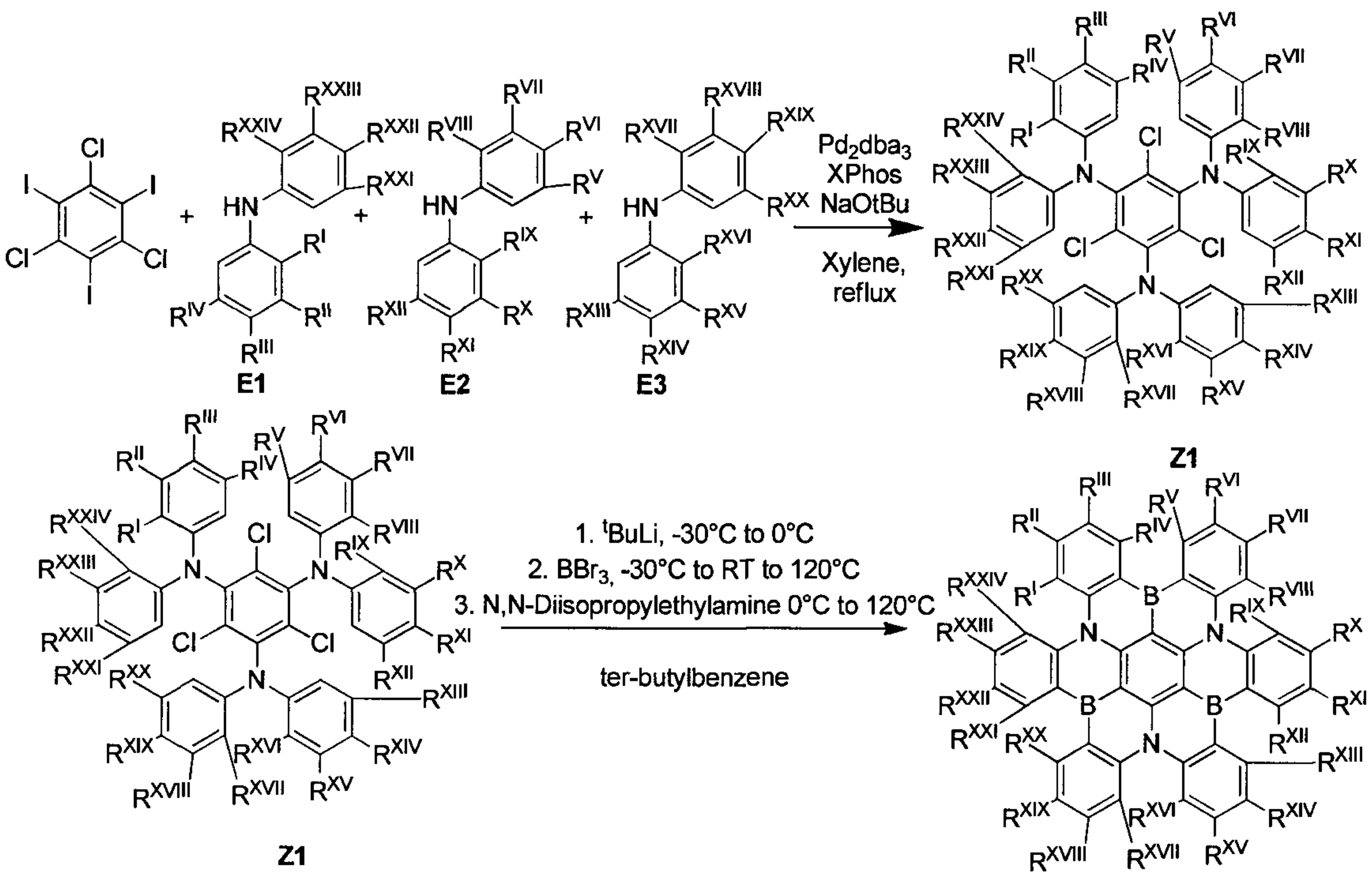
- prepared by means of an organic vapor phase deposition process,
- prepared by means of a carrier gas sublimation process,
- solution processed or printed.

The methods used to fabricate the organic electroluminescent 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.

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 exemplarily 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 optionally be completely or partially removed by means known in the state of the art.

Examples

General synthesis scheme I



P1

General procedure for synthesis:

1,3,5-Trichloro-2,4,6-triiodobenzene (1 equivalent), **E1** (1.33 equivalents), **E2** (1.33 equivalents) and **E3** (1.33 equivalents) Pd_2dba_3 (0.06 equivalents), XPhos (0.12 equivalents) and potassium phosphate tribasic (6.0 equivalents) are added into a reaction vessel, vacuum and backfilled with argon. Dry xylene was added, the mixture degassed for 15 min and then heated to reflux under argon for 48h. Activated charcoal and celite were added to the hot mixture and stirred for 15 minutes. The mixture is then cooled down to 50-60°C, vacuum filtered and washed with hot toluene. The solvent is evaporated and the residue recrystallized from ethanol/chloroform to afford **Z1** as a solid.

Z1 (1.00 equivalents) was dissolved in tert-butylbenzene and the solution was cooled to -30 °C. tert-Butyllithium (^{t}BuLi) (6.00 equivalents) was added dropwise and the reaction mixture was allowed to warm up to 0 °C. After stirring for 30 minutes at 0 °C, the reaction mixture was cooled again to -30 °C.

A solution of boron tribromide (BBr_3, 3.3 equivalents) was added dropwise, the bath was removed and the reaction mixture was allowed to warm up to room temperature (rt). Subsequently, the reaction mixture was heated at reflux at 120 °C for 12h. The solution was cooled to 0 °C, N,N-diisopropylethylamine (8.00 equivalents) was added and the solution heated again to 120 °C for 6 hours. Volatiles were removed under reduced pressure, the residue dissolved in toluene and filtered through a silica gel column. The filtrate was dried and evaporated under vacuum to obtain **P1**.

Cyclic voltammetry

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 SCE.

Density functional theory calculation

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.

Photophysical measurements

Sample pretreatment: Spin-coating
Apparatus: Spin150, SPS euro.
The sample concentration is 10 mg/ml, dissolved in a suitable solvent.
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.

Photoluminescence spectroscopy and TCSPC (*Time-correlated single-photon counting*)
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.

Excited state lifetimes are determined employing the same system using the TCSPC method with FM-2013 equipment and a Horiba Yvon TCSPC hub.
Excitation sources:
NanoLED 370 (wavelength: 371 nm, puls duration: 1,1 ns)
NanoLED 290 (wavelength: 294 nm, puls duration: <1 ns)
SpectraLED 310 (wavelength: 314 nm)
SpectraLED 355 (wavelength: 355 nm).

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

Photoluminescence quantum yield measurements
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.
Emission maxima are given in nm, quantum yields Φ in % and CIE coordinates as x,y values.
PLQY is determined using the following protocol:

1) Quality assurance: Anthracene in ethanol (known concentration) is used as reference
2) Excitation wavelength: the absorption maximum of the organic molecule is determined and the molecule is excited using this wavelength
3) Measurement

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

$$\Phi_{PL} = \frac{n_{photon}, emited}{n_{photon}, absorbed} = \frac{\int \frac{\lambda}{c}\left[Int_{emitted}^{sample}(\lambda) \quad Int_{absorbed}^{sample}(\lambda)\right]d\lambda}{\int \frac{\lambda}{c}\left[Int_{emitted}^{reference}(\lambda) \quad Int_{absorbed}^{reference}(\lambda)\right]d\lambda}$$

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

Production and characterization of organic electroluminescence devices

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 %.

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.

Accelerated lifetime measurements are performed (e.g. applying increased current densities). Exemplarily LT80 values at 500 cd/m² are determined using the following equation:

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

wherein L_0 denotes the initial luminance at the applied current density.

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

HPLC-MS:

HPLC-MS spectroscopy is performed on a HPLC by Agilent (1100 series) with MS-detector (Thermo LTQ XL). A reverse phase column 4.6 mm x 150 mm, particle size 5.0 µm from Waters (without pre-column) is used in the HPLC. The HPLC-MS measurements are performed at room temperature (rt) with the solvents acetonitrile, water and THF in the following concentrations:

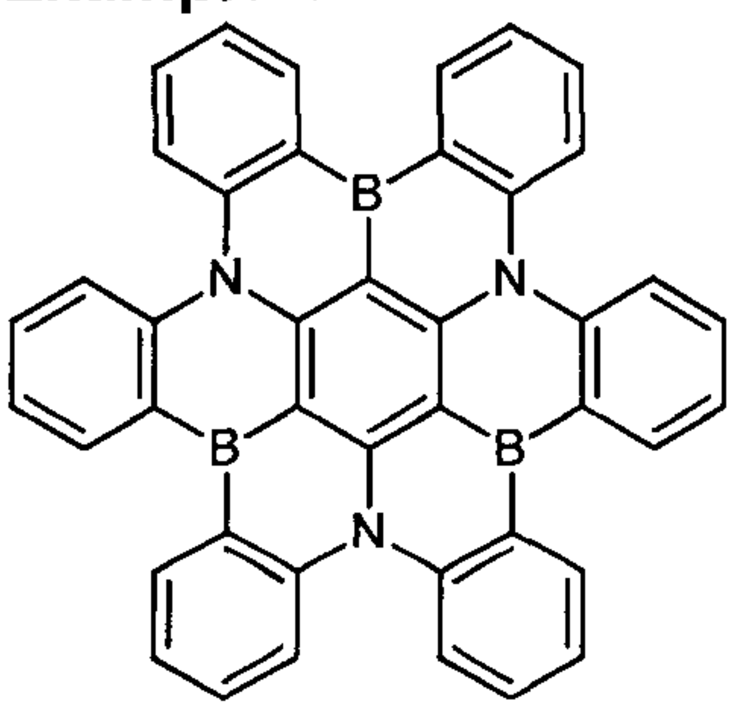
solvent A:	H_2O (90%) MeCN (10%)
solvent B:	H_2O (10%) MeCN (90%)
solvent C:	THF (100%)

From a solution with a concentration of 0.5mg/ml an injection volume of 15 µL is taken for the measurements. The following gradient is used:

Flow rate [ml/min]	time [min]	A[%]	B[%]	D[%]
3	0	40	50	10
3	10	10	15	75
3	16	10	15	75
3	16.01	40	50	10
3	20	40	50	10

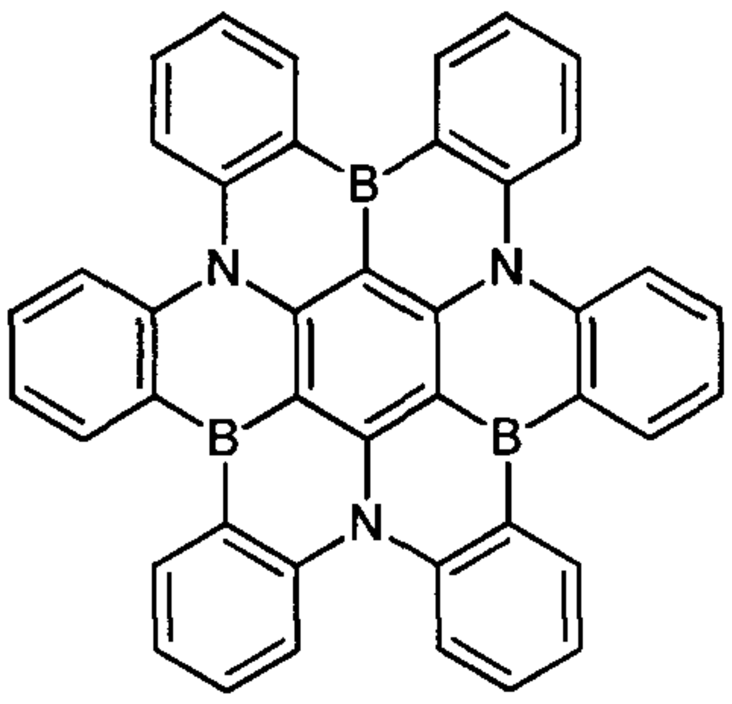
Ionisation of the probe is performed by APCI (atmospheric pressure chemical ionization).

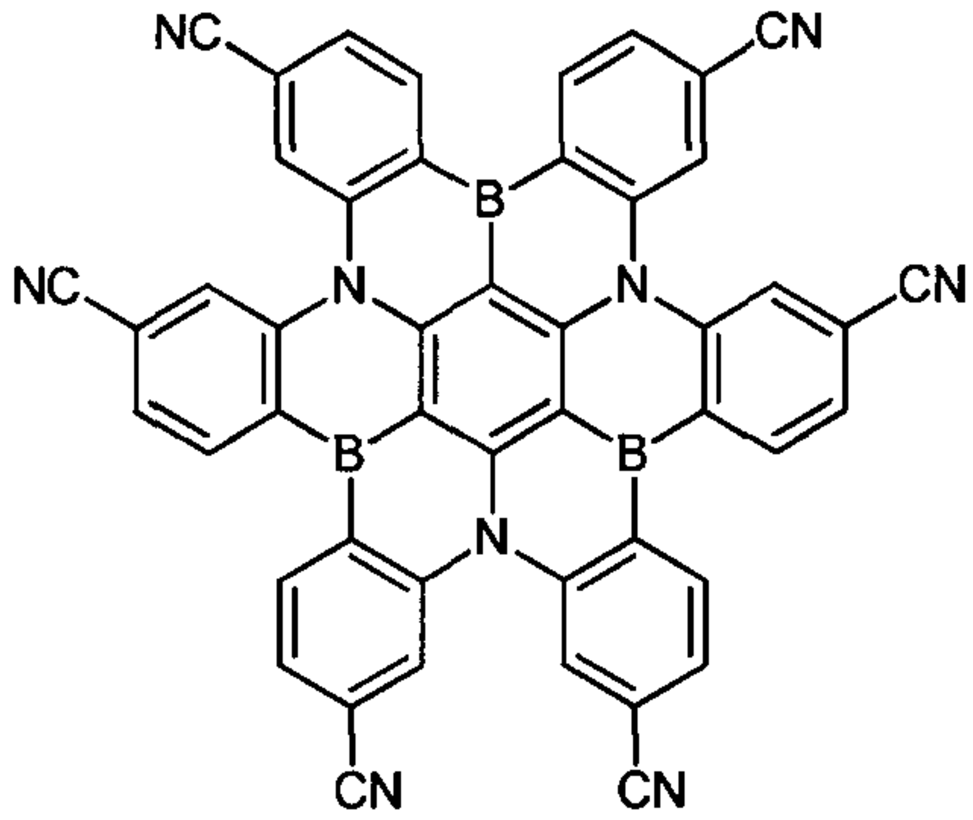
Example 1

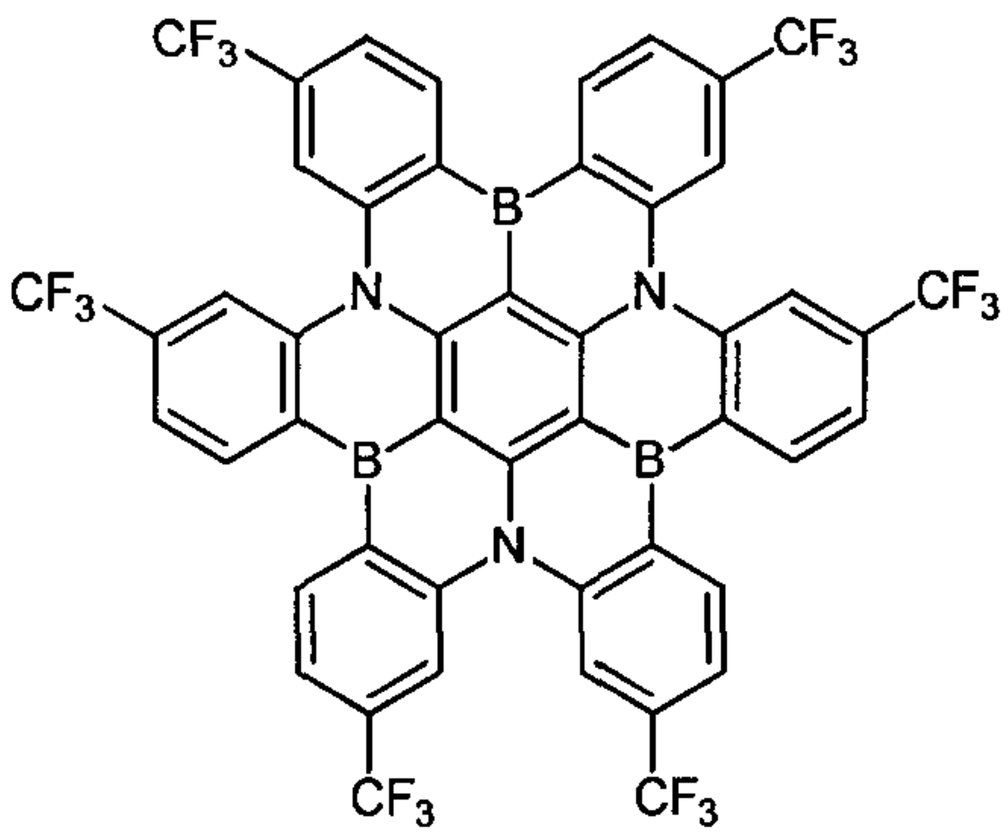


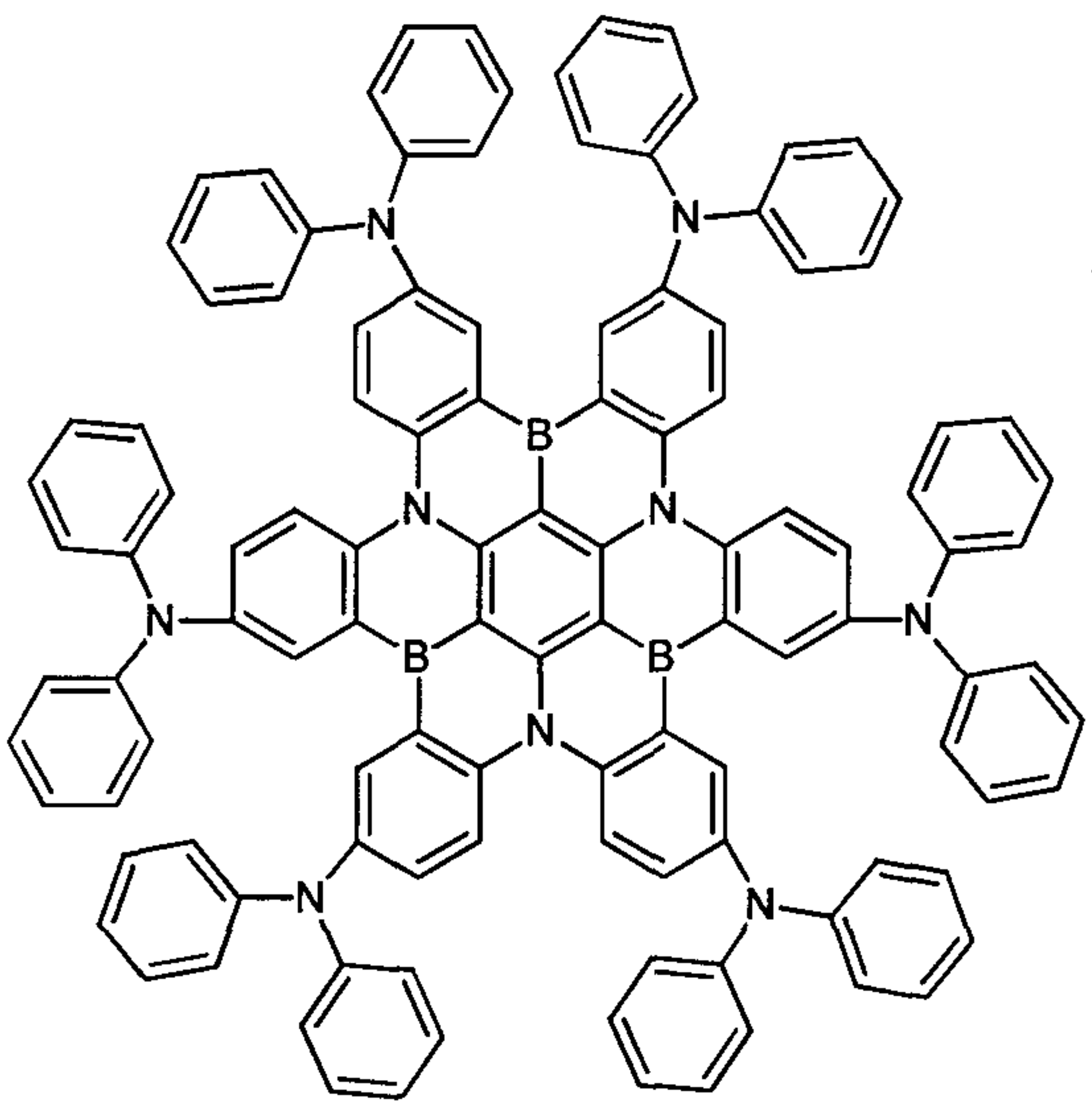
Example **1** was synthesized according to the general procedure for synthesis, wherein diphenylamine (**E1**, **E2** and **E3**), was used as reactant.

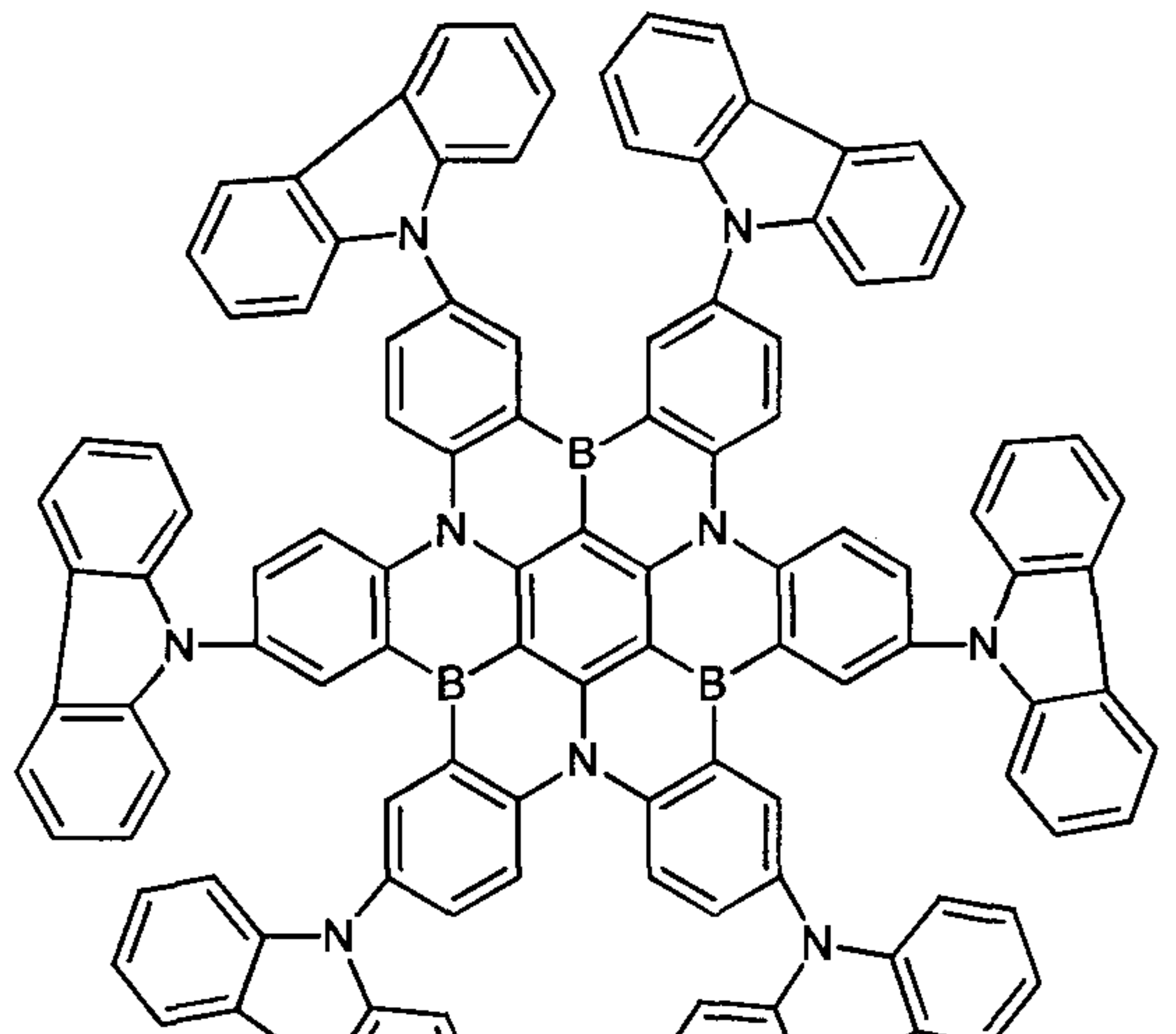
Additional Examples of organic molecules of the invention

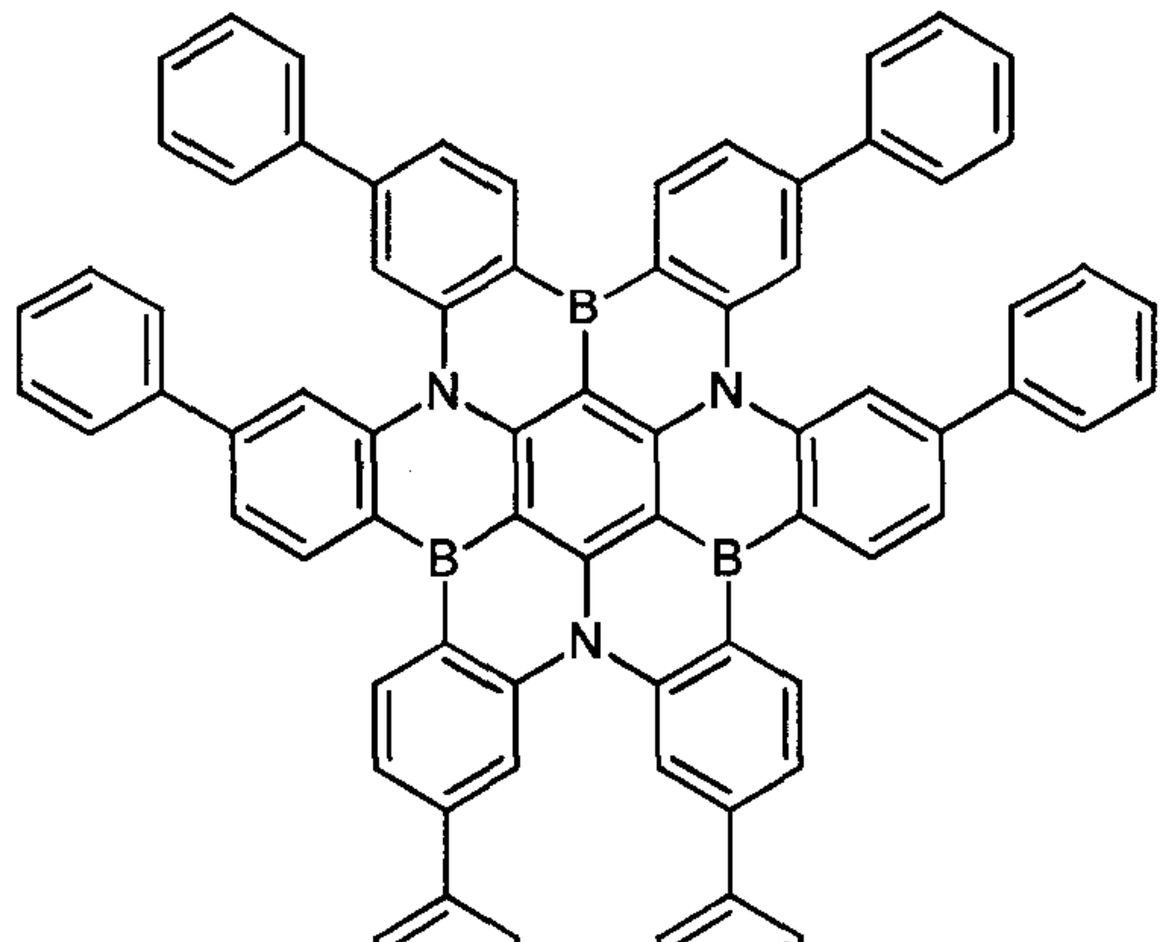


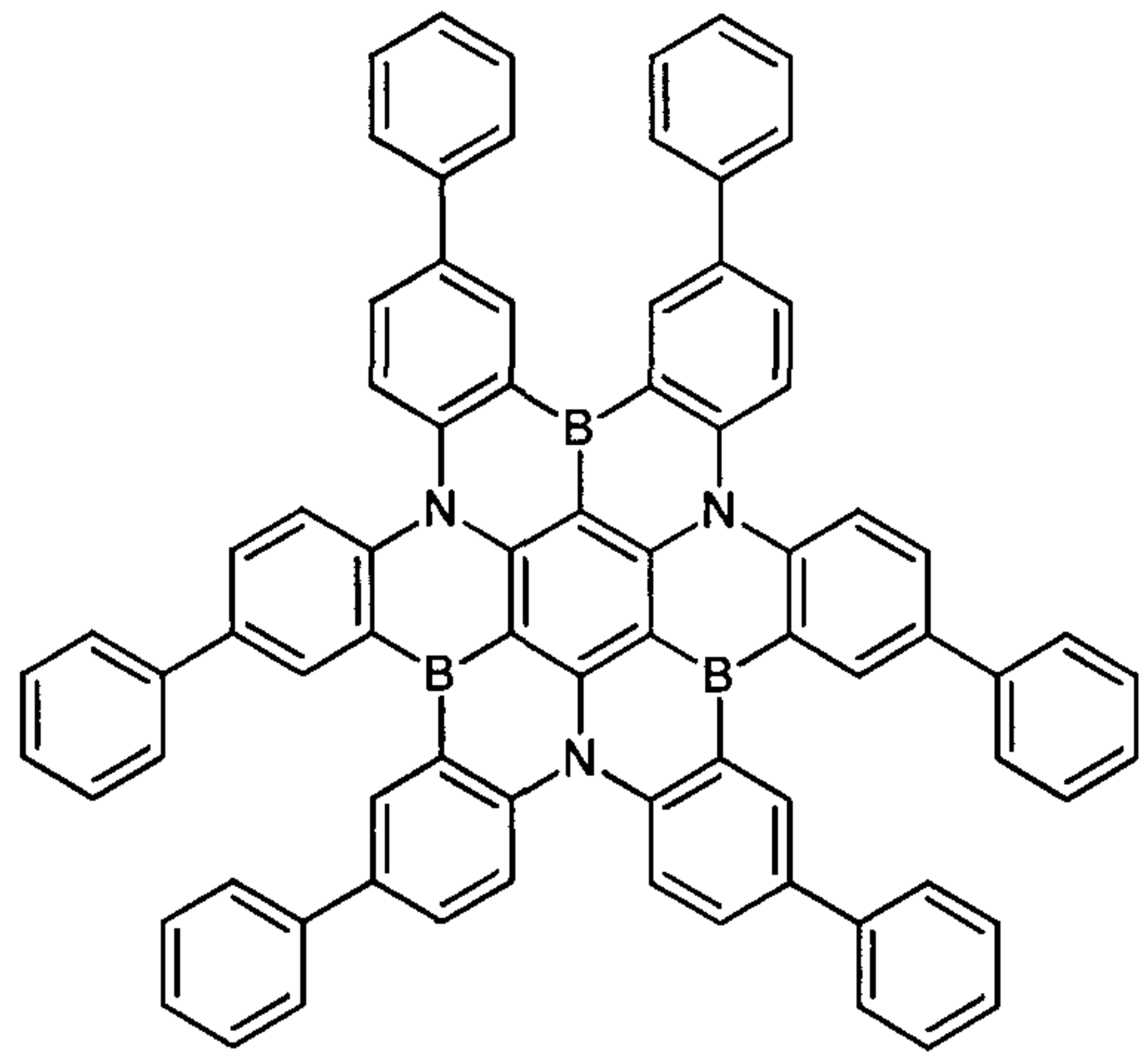


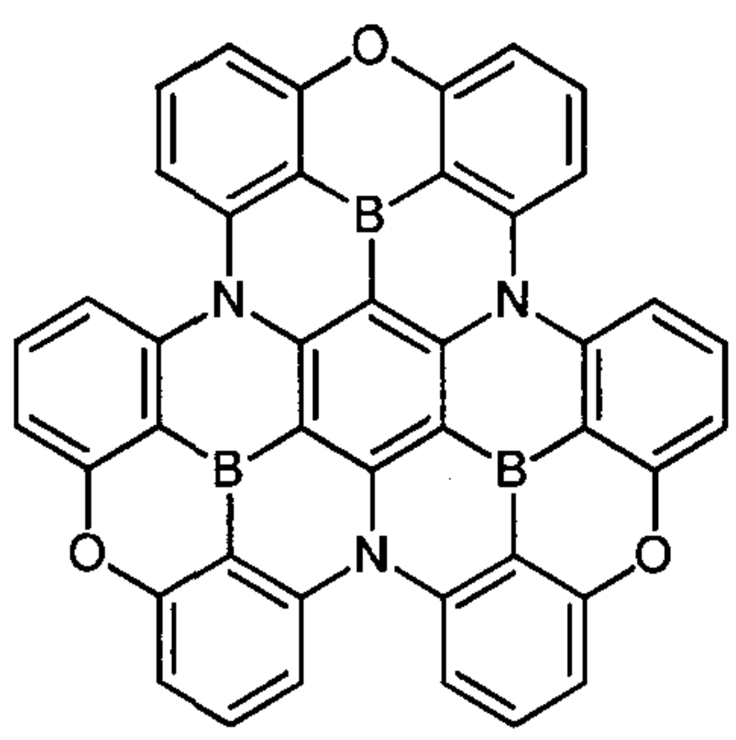


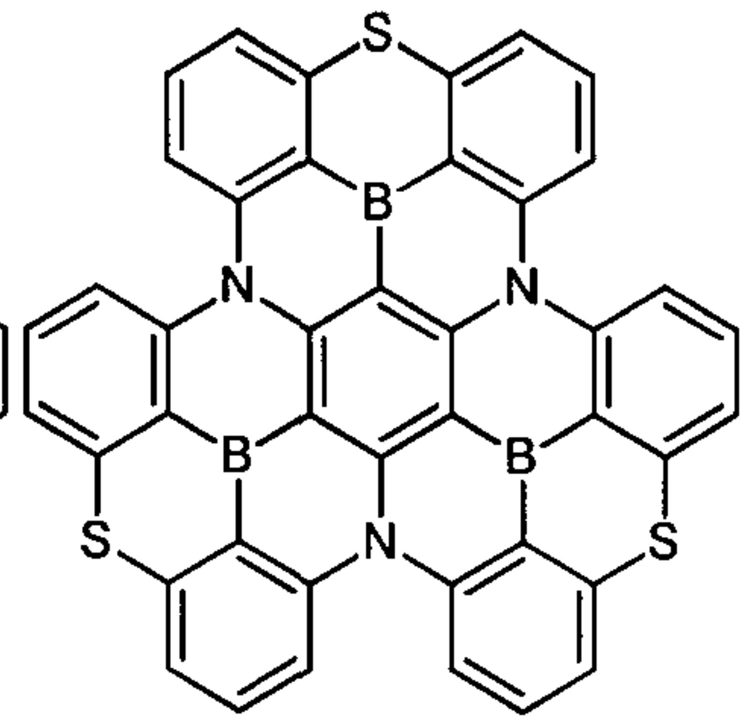


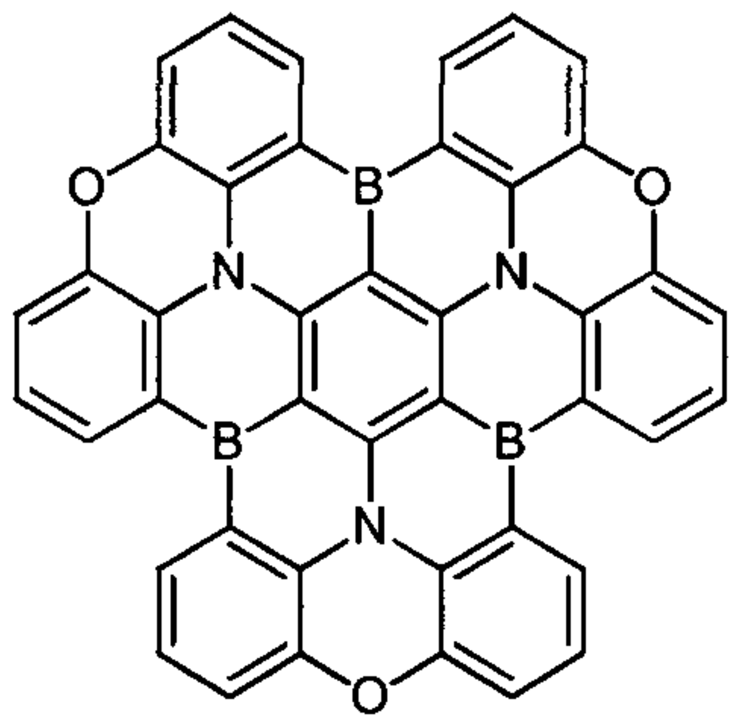


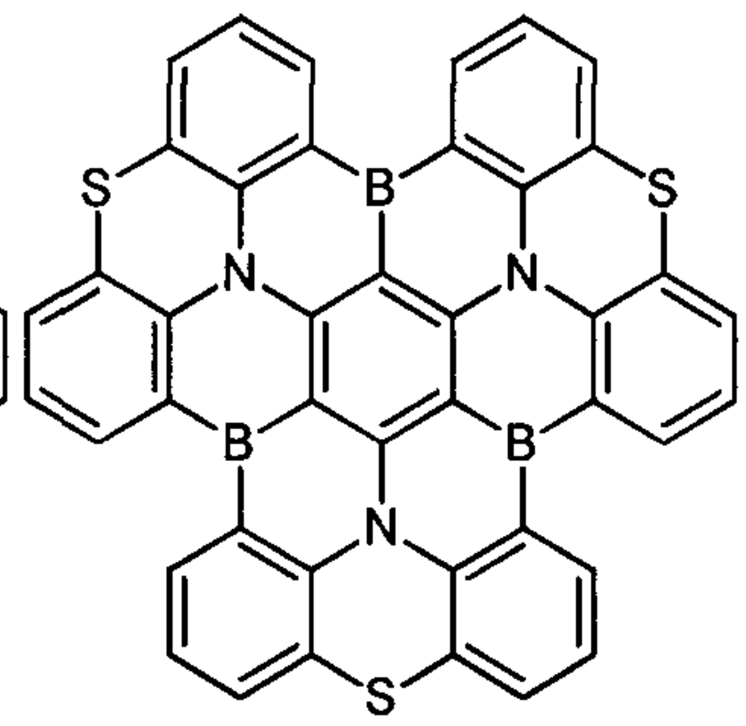






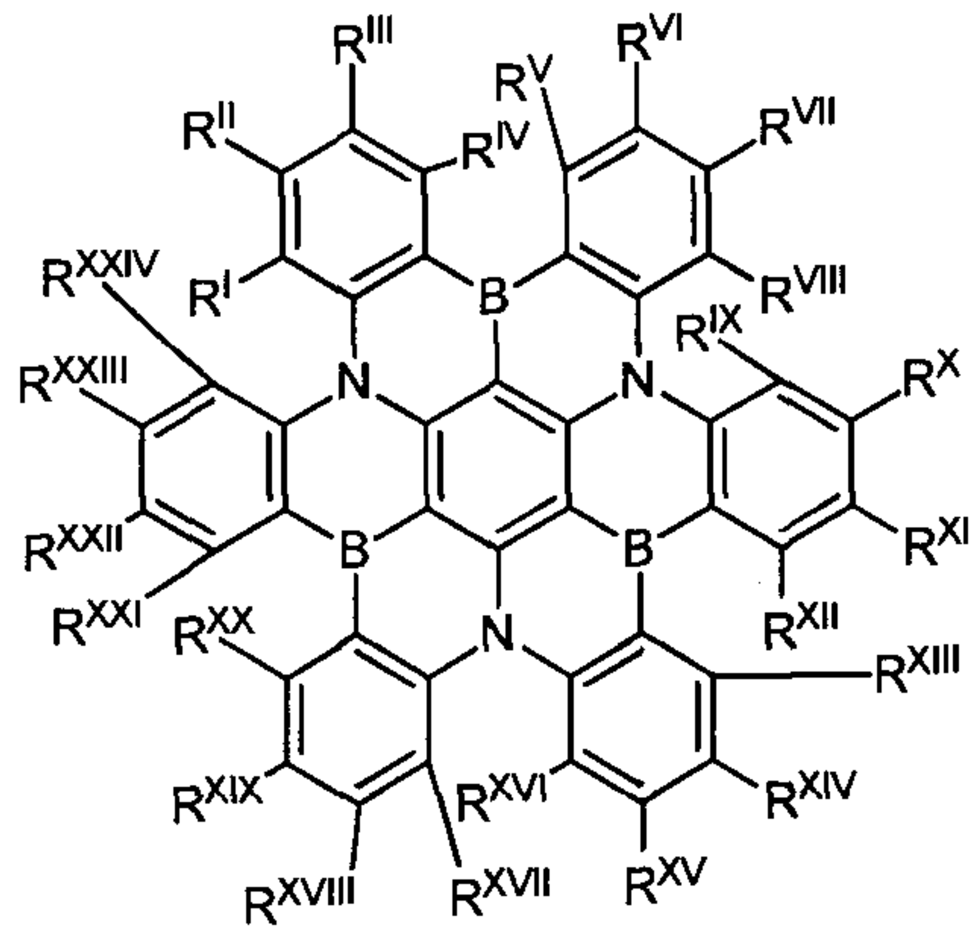






Claims

1. Organic molecule with a structure of Formula I,



Formula I

wherein

R^{I}, R^{II}, R^{III}, R^{IV}, R^{V}, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^{X}, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} is independently from each other selected from the group consisting of:

hydrogen,

deuterium,

C_1-C_{40}-alkyl,

which is optionally substituted with one or more substituents R^1;

C_1-C_{40}-alkoxyl,

which is optionally substituted with one or more substituents R^1;

C_2-C_{40}-alkenyl,

which is optionally substituted with one or more substituents R^1;

C_2-C_{40}-alkynyl,

which is optionally substituted with one or more substituents R^1;

C_6-C_{60}-aryl,

which is optionally substituted with one or more substituents R^1;

C_3-C_{57}-heteroaryl,

which is optionally substituted with one or more substituents R^1;

CN;

CF_3;

$N(R^1)_2$;

OR^1, and
$Si(R^1)_3$;

R^1 is at each occurrence independently from another selected from the group consisting of: hydrogen, deuterium, OPh, CF_3, CN, F,

C_1-C_5-alkyl,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_1-C_5-alkoxy,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_1-C_5-thioalkoxy,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_2-C_5-alkenyl,

wherein optionally one or more hydrogen atoms are independently from each other substituted by deuterium, CN, CF_3, or F;

C_2-C_5-alkynyl,

wherein optionally one or more hydrogen atoms are independently from each other 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_3-C_{17}-heteroaryl,

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

$N(C_6$-C_{18}-aryl$)_2$,
$N(C_3$-C_{17}-heteroaryl$)_2$; and
$N(C_3$-C_{17}-heteroaryl$)(C_6$-C_{18}-aryl$)$;

wherein at least one substituent selected from R^I, R^{II}, R^{III}, R^{IV}, R^V, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^X, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} independently from each other optionally forms a mono- or polycyclic, aliphatic, aromatic and/or benzo-fused ring system with one or more substituents R^I, R^{II}, R^{III}, R^{IV}, R^V, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^X, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV}.

2. Organic molecule according to claim 1, wherein R^{I}, R^{II}, R^{III}, R^{IV}, R^{V}, R^{VI}, R^{VII}, R^{VIII}, R^{IX}, R^{X}, R^{XI}, R^{XII}, R^{XIII}, R^{XIV}, R^{XV}, R^{XVI}, R^{XVII}, R^{XVIII}, R^{XIX}, R^{XX}, R^{XXI}, R^{XXII}, R^{XXIII} and R^{XIV} is independently from another selected from the group consisting of:

hydrogen,

deuterium,

halogen,

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 $N(Ph)_2$.

3. Organic molecule according to claim 1 or 2, wherein R^{II}, R^{IV}, R^{VI}, R^{VIII}, R^{X}, R^{XII}, R^{XIV}, R^{XVI}, R^{XVIII}, R^{XX}, R^{XXII} and R^{XXIV} is independently from another selected from the group consisting of:

hydrogen,

deuterium,

halogen,

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, and

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;

R^{I}, R^{III}, R^{V}, R^{VII}, R^{IX}, R^{XI}, R^{XIII}, R^{XV}, R^{XVII}, R^{XIX}, R^{XXI} and R^{XXIII} is independently from another selected from the group consisting of:

hydrogen,

deuterium,

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, 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,

and $N(Ph)_2$.

4. Organic molecule according to claim 3, wherein

- R^{II}, R^{IV}, R^{VI}, R^{VIII}, R^{X}, R^{XII}, R^{XIV}, R^{XVI}, R^{XVIII}, R^{XX}, R^{XXII} and R^{XXIV} is independently from another selected from the group consisting of:

hydrogen, deuterium, Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and

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;

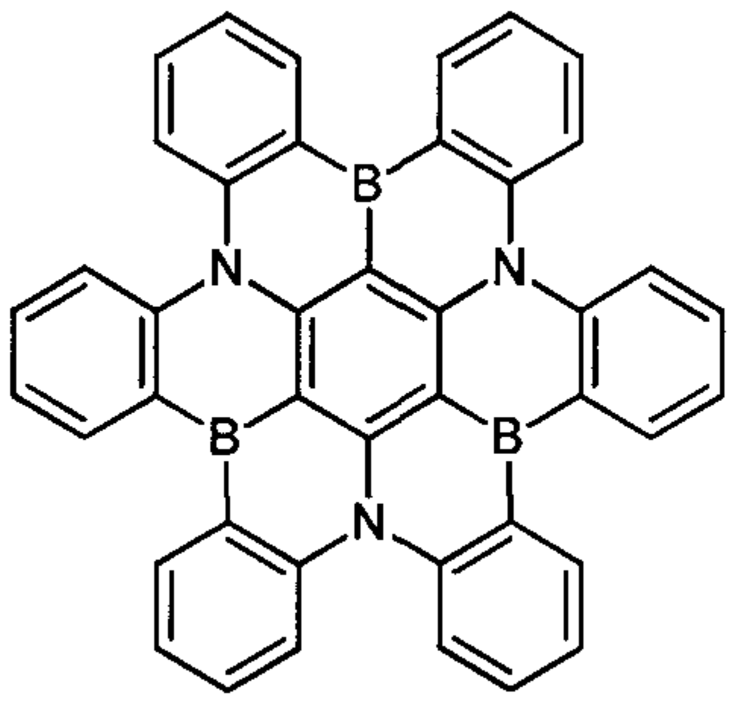
- R^{I}, R^{III}, R^{V}, R^{VII}, R^{IX}, R^{XI}, R^{XIII}, R^{XV}, R^{XVII}, R^{XIX}, R^{XXI} and R^{XXIII} is independently from another selected from the group consisting of hydrogen, deuterium, Me, ^{i}Pr, ^{t}Bu,

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, and Ph,

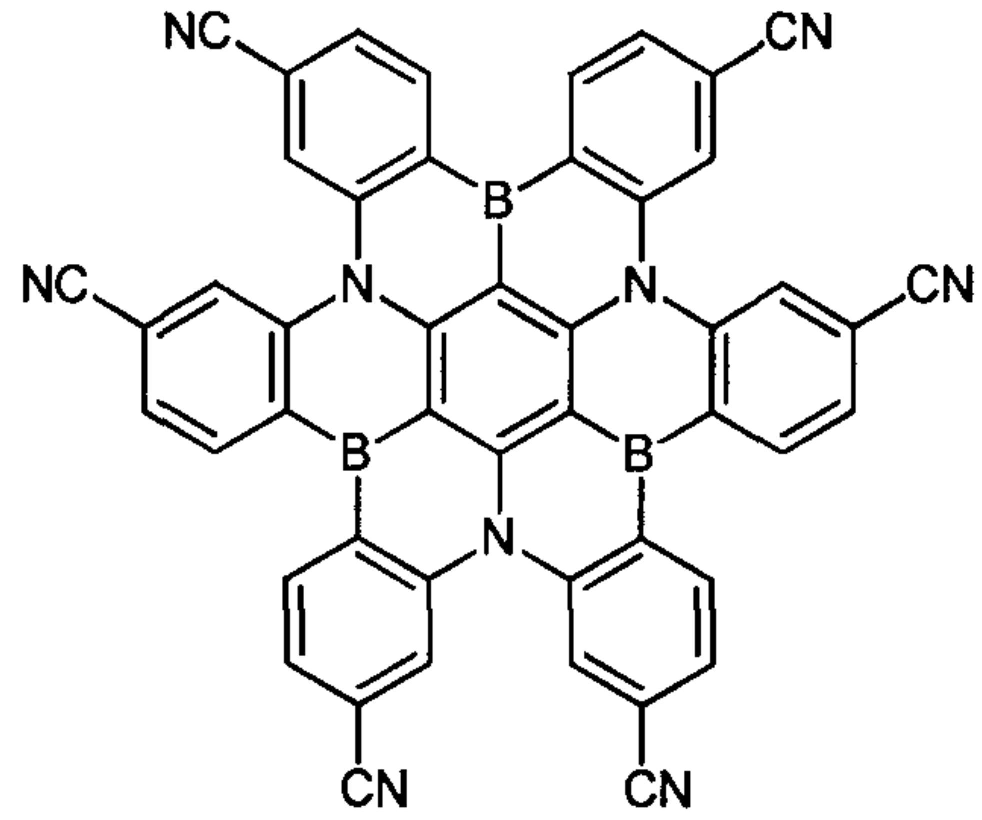
carbazolyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{t}Bu, and Ph

and $N(Ph)_2$.

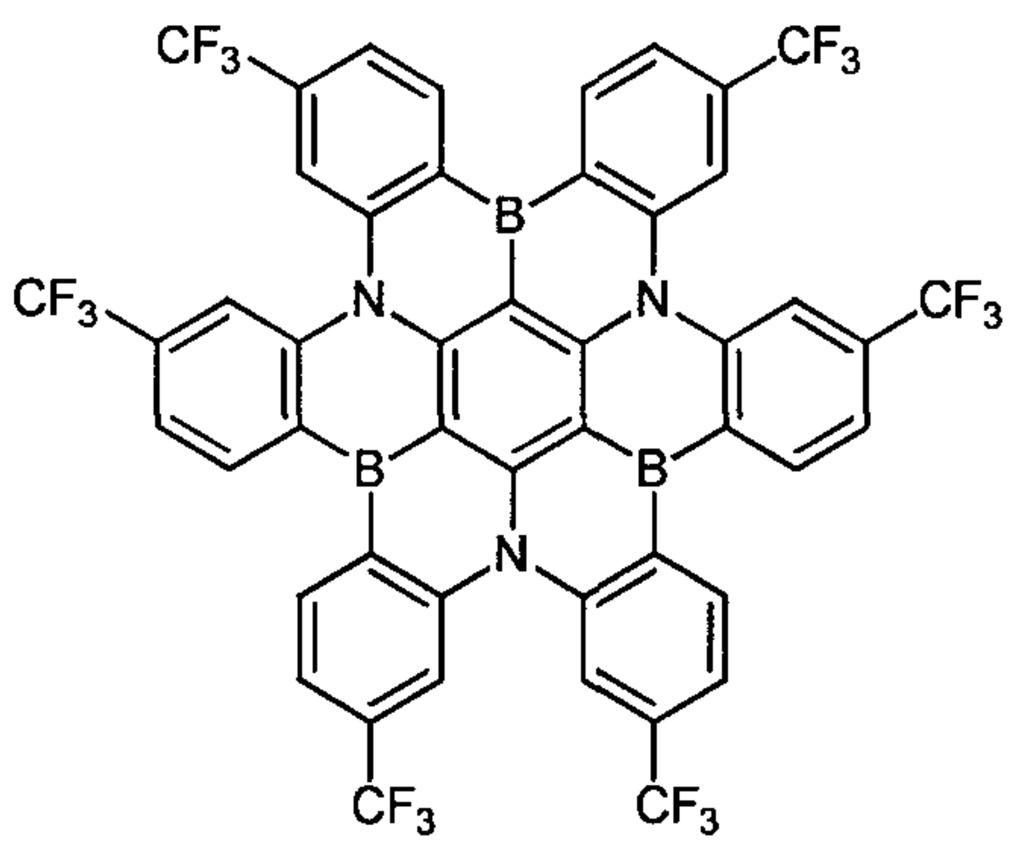
5. Organic molecule according to claim 1, with a structure of one of Formulas II to IX:



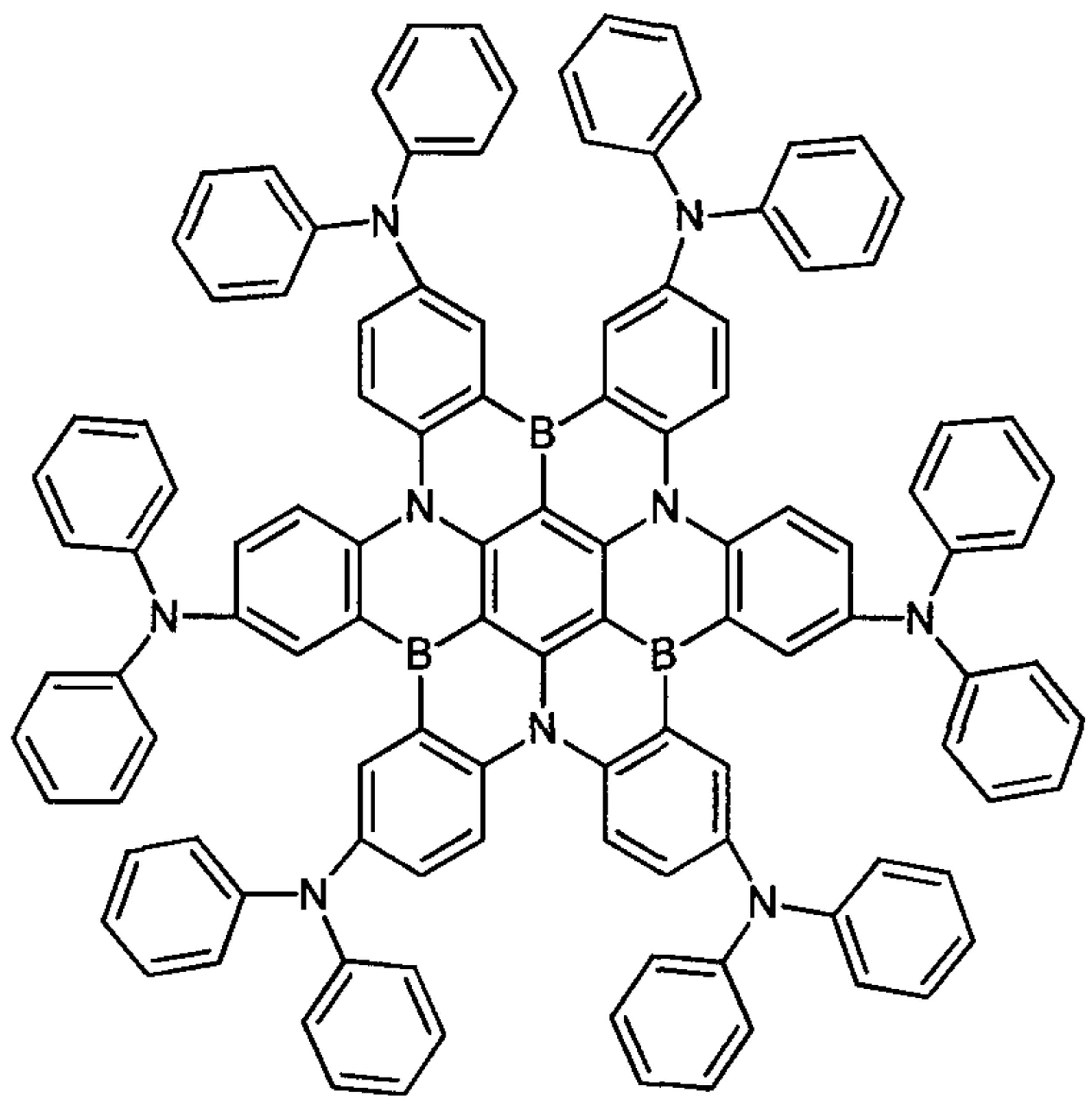
Formula II



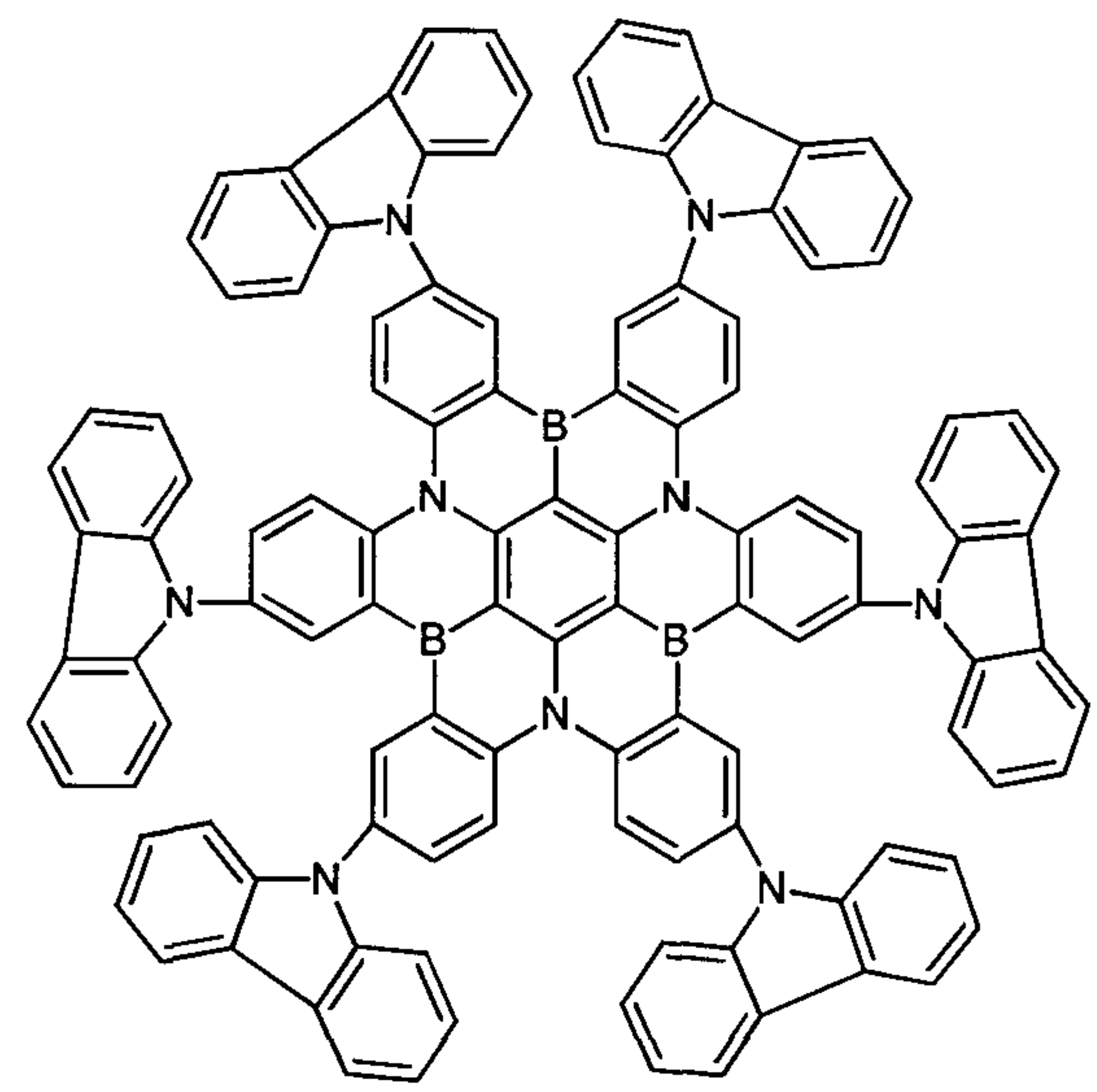
Formula III

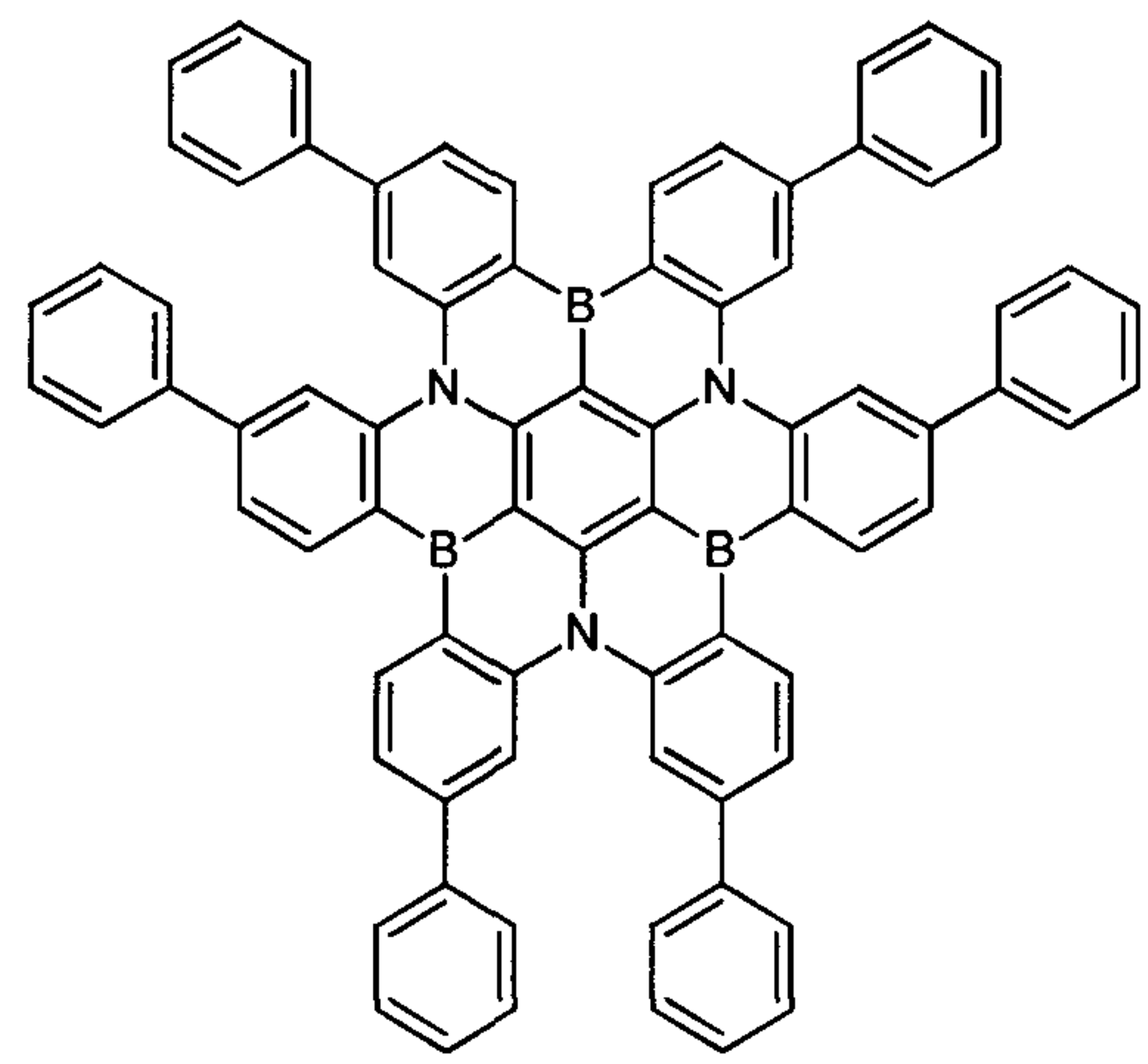


Formula V



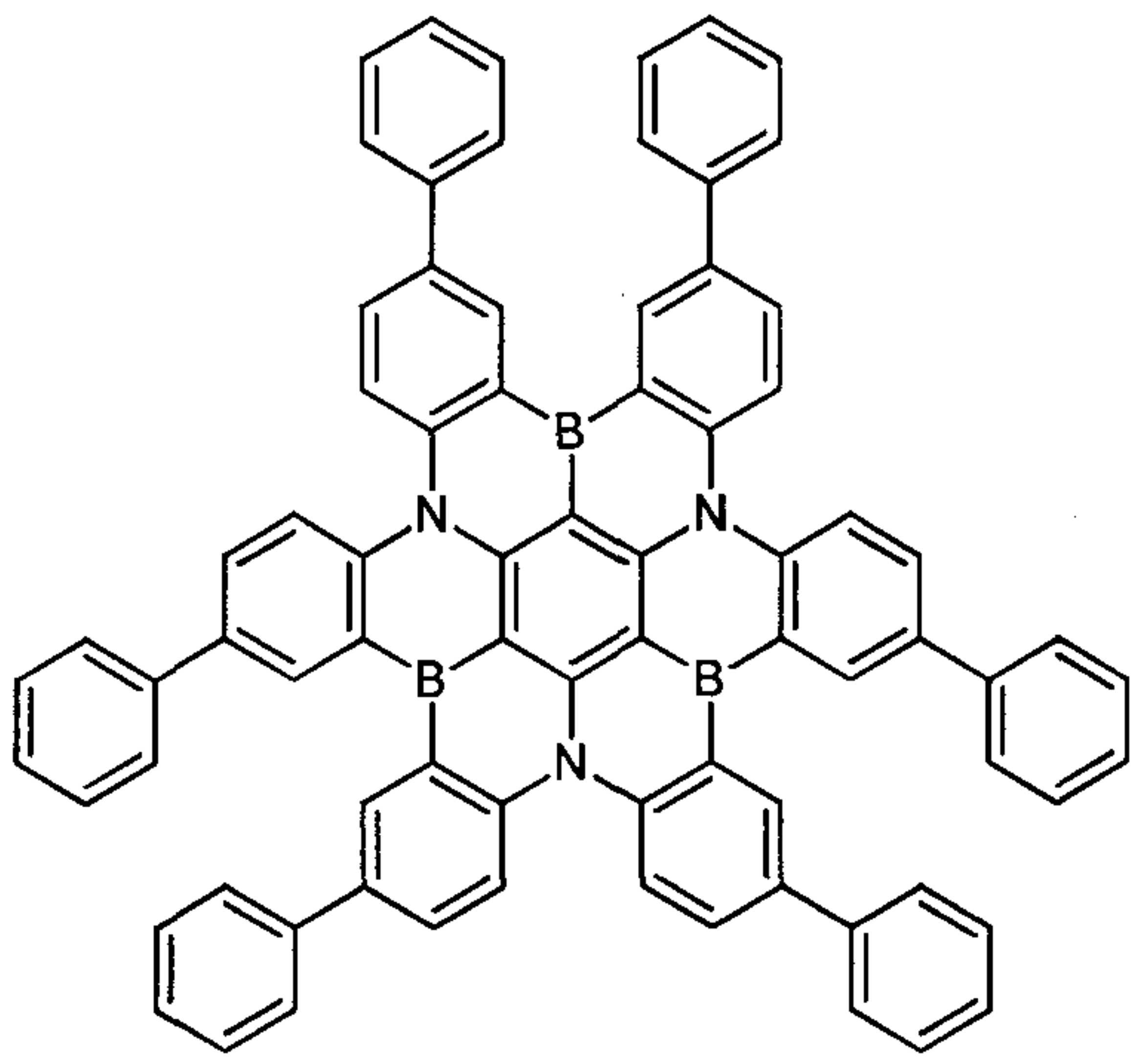
Formula VI





Formula VII

Formula VIII



Formula IX

6. Use of an organic molecule according to one or more of claims 1 to 5 as a luminescent emitter in an optoelectronic device.

7. Use according to claim 6, wherein the optoelectronic device is selected from the group consisting of:

- organic light-emitting diodes (OLEDS),
- light-emitting electrochemical cells,
- OLED-sensors,
- organic diodes,
- organic solar cells,
- organic transistors,
- organic field-effect transistors,
- organic lasers, and
- down-conversion elements.

8. Composition, comprising or consisting of:

(a) at least one organic molecule according to one or more of claims 1 to 5, in particular in the form of an emitter and/or a host, and

(b) one or more emitter and/or host materials, which differ from the organic molecule of one or more of claims 1 to 5, and

(c) optionally, one or more dyes and/or one or more solvents.

9. Optoelectronic device, comprising an organic molecule according to one or more of claims 1 to 5 or a composition according to claim 8, in particular in form of a device selected from the group consisting of organic light-emitting diode (OLED), light-emitting electrochemical cell, OLED-sensor, organic diode, organic solar cell, organic transistor, organic field-effect transistor, organic laser and down-conversion element.

10. Optoelectronic device according to claim 10, comprising or consisting of:
- a substrate,
- an anode, and
- a cathode, wherein the anode or the cathode are disposed on the substrate, and
- at least one light-emitting layer, which is arranged between anode and cathode and which comprises the organic molecule according to claims 1 to 5 or a composition according to claim 8.

11. Process for producing an optoelectronic device, wherein an organic molecule according to any one of claims 1 to 5 or a composition according to claim 8 is used, in particular comprising the processing of the organic compound by a vacuum evaporation method or from a solution.