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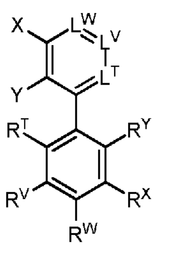
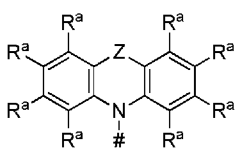


Formula I



Formula II

(57) **Abstract:** The invention relates to an organic compound, in particular for the application in optoelectronic devices. According to the invention, the organic compound consists of - one first chemical moiety with a structure of formula I, and - one second chemical moiety comprising or consisting of a structure of Formula II, wherein the first chemical moiety is linked to the second chemical moiety via a single bond; wherein L^T is N or C-T; L^V is N or C-V; L^W is N or C-W; exactly one ring atom selected from the group consisting of L^T, L^V and L^W is N; exactly one substituent selected from the group consisting of R^T, R^V, R^W, R^X and R^Y is R^A; exactly one substituent selected from the group consisting of T, V, W, X and Y is R^A; and exactly one substituent selected from the group consisting of R^W, R^Y and R^X represents the binding site of a single bond linking the first chemical moiety and the second chemical moiety.

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ORGANIC MOLECULES
FOR USE IN OPTOELECTRONIC DEVICES

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

Description

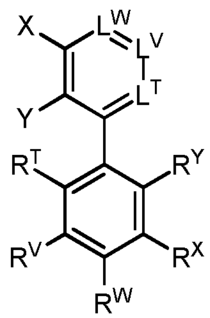
The object of the present invention is to provide molecules which are suitable for use in optoelectronic devices.

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, 50 % or more. The molecules according to the invention exhibit in particular thermally activated delayed fluorescence (TADF). 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 of the device. Corresponding OLEDs have a higher stability than OLEDs with known emitter materials and comparable color.

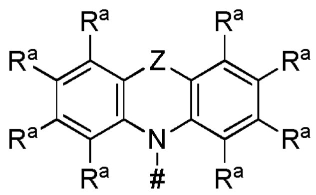
The organic light-emitting molecules of the invention comprise or consist of one first chemical moiety comprising or consisting of a structure of Formula I,



Formula I

and

- one second chemical moiety comprising or consisting of a structure of Formula II,



Formula II

wherein the first chemical moiety is linked to the second chemical moiety via a single bond.

L^T is N or C-T.

L^V is N or C-V.

L^W is N or C-W.

T is selected from the group consisting of R^A and R^1.

V is selected from the group consisting of R^A and R^1.

W is selected from the group consisting of R^A and R^1.

X is selected from the group consisting of R^A and R^2.

Y is selected from the group consisting of R^A and R^2.

R^T is selected from the group consisting of R^A and R^I.

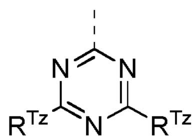
R^V is selected from the group consisting of R^A and R^I.

R^W is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I.

R^X is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I.

R^Y is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I.

R^A comprises or consists a structure of Formula Tz:



Formula Tz

wherein the dotted bond represents the binding site of R^A to the single bond linking the first chemical moiety and R^A.

represents the binding site of a single bond linking the second chemical moiety to the first chemical moiety;

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

R^1 is at each occurrence independently from another selected from the group consisting of
hydrogen,
deuterium,
C_1-C_5-alkyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_2-C_8-alkenyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_2-C_8-alkynyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium; and
C_6-C_{18}-aryl,
which is optionally substituted with one or more substituents R^6.

R^2 is at each occurrence independently from another selected from the group consisting of
hydrogen,
deuterium,
C_1-C_5-alkyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_2-C_8-alkenyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_2-C_8-alkynyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium; and
C_6-C_{18}-aryl,
which is optionally substituted with one or more substituents R^6.

R^I is at each occurrence independently from another selected from the group consisting of
hydrogen,
deuterium,
C_1-C_5-alkyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_2-C_8-alkenyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_2-C_8-alkynyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium; and
C_6-C_{18}-aryl,
which is optionally substituted with one or more substituents R^6.

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

hydrogen,
deuterium,
C_1-C_5-alkyl,
wherein one or more hydrogen atoms are optionally substituted by deuterium;
C_6-C_{18}-aryl,
which is optionally substituted with one or more substituents R^6, and
C_3-C_{17}-heteroaryl,
which is optionally substituted with one or more substituents R^6.

R^a, R^3 and R^4 is at each occurrence independently from another selected from the group consisting of hydrogen, deuterium, $N(R^5)_2$, OR^5, $Si(R^5)_3$, $B(OR^5)_2$, OSO_2R^5, CF_3, CN, F, Br, I,
C_1-C_{40}-alkyl,
which is optionally substituted with one or more substituents R^5 and
wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C{=}CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C{=}NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;
C_1-C_{40}-alkoxy,
which is optionally substituted with one or more substituents R^5 and
wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C{=}CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C{=}NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;
C_1-C_{40}-thioalkoxy,
which is optionally substituted with one or more substituents R^5 and
wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C{=}CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C{=}NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;
C_2-C_{40}-alkenyl,
which is optionally substituted with one or more substituents R^5 and
wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C{=}CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C{=}NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;
C_2-C_{40}-alkynyl,
which is optionally substituted with one or more substituents R^5 and
wherein one or more non-adjacent CH_2-groups are optionally substituted by $R^5C{=}CR^5$, C≡C, $Si(R^5)_2$, $Ge(R^5)_2$, $Sn(R^5)_2$, C=O, C=S, C=Se, $C{=}NR^5$, $P(=O)(R^5)$, SO, SO_2, NR^5, O, S or $CONR^5$;
C_6-C_{60}-aryl,

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

C_3-C_{57}-heteroaryl,

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

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

C_1-C_{40}-alkyl,

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

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

C_1-C_{40}-alkoxy,

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

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

C_1-C_{40}-thioalkoxy,

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

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

C_2-C_{40}-alkenyl,

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

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

C_2-C_{40}-alkynyl,

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

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

C_6-C_{60}-aryl,

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

C_3-C_{57}-heteroaryl,

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

R^6 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)$_2$,

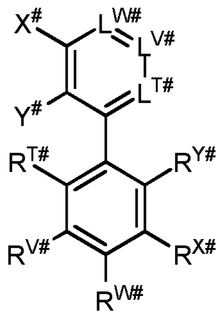
N(C_3-C_{17}-heteroaryl)$_2$; and

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

The substituents R^a, R^3, R^4 or R^5 independently from each other can optionally form a mono- or polycyclic, aliphatic, aromatic and/or benzo-fused ring system with one or more substituents R^a, R^3, R^4 or R^5.

According to the invention exactly one (one and only one) ring member (atom or group) selected from the group consisting of L^T, L^V and L^W is N; exactly one substituent selected from the group consisting of R^T, R^V, R^W, R^X and R^Y is R^A, exactly one substituent selected from the group consisting of T, V, W, X and Y is R^A and exactly one substituent selected from the group consisting of R^W, R^Y and R^X represents the binding site of a single bond linking the first chemical moiety and the second chemical moiety.

In one embodiment of the invention, first chemical moiety comprises or consists of a structure of Formula Ia:



Formula Ia

wherein R^1, R^2, R^I and R^A are defined as above;

$L^{T\#}$ is N or C-R^1;

$L^{V\#}$ is N or C- R^1,

$L^{W\#}$ is N or C-$W^\#$;

$W^\#$ is selected from the group consisting of R^A and R^1;

$X^\#$ is selected from the group consisting of R^A and R^2;

$Y^\#$ is selected from the group consisting of R^A and R^2;

$R^{T\#}$ is selected from the group consisting of R^A and R^I;

$R^{V\#}$ is selected from the group consisting of R^A and R^I;

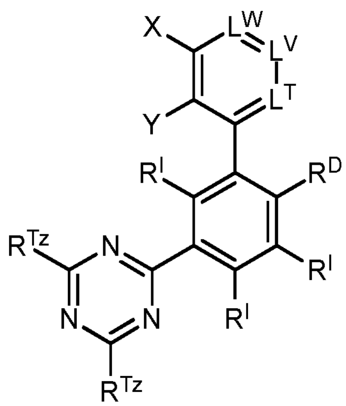
$R^{W\#}$ is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I;

$R^{X\#}$ is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is R^I;

$R^{Y\#}$ is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is R^I;

wherein exactly one ring member (atom or group) selected from the group consisting of $L^{T\#}$, $L^{V\#}$ and $L^{W\#}$ is N; exactly one substituent selected from the group consisting of $R^{T\#}$, $R^{V\#}$ and $R^{W\#}$ is R^A, exactly one substituent selected from the group consisting of $W^\#$, $X^\#$ and $Y^\#$ is R^A and exactly one substituent selected from the group consisting of $R^{W\#}$, $R^{Y\#}$ and $R^{X\#}$ represents the binding site of a single bond linking the first chemical moiety and the second chemical moiety.

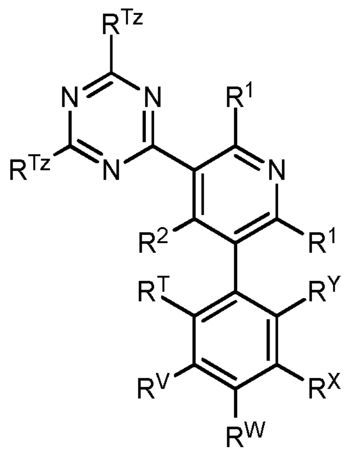
In one embodiment of the invention, first chemical moiety comprises or consists of a structure of Formula Iaa:



Formula Iaa

wherein L^T, L^V, L^W, X, Y, R^I and and R^{Tz} are defined as above;
R^D is the binding site of a single bond linking the first chemical moiety to the second chemical moiety.

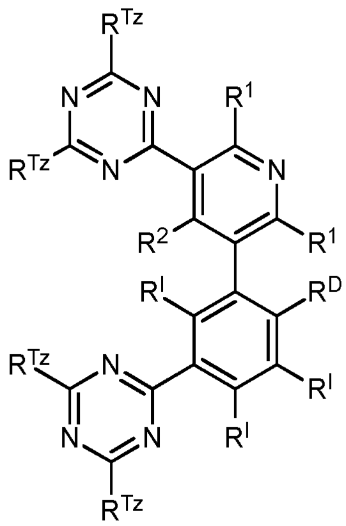
In one embodiment of the invention, first chemical moiety comprises or consists of a structure of Formula Iaaa:



Formula Iaaa

wherein R^T, R^V, R^W, R^X, R^Y, R^1, R^2 and R^{Tz} are defined as above;
exactly one substituent selected from the group consisting of R^T, R^V, R^W, R^X and R^Y is R^A;
and exactly one substituent selected from the group consisting of R^W, R^Y and R^X represents the binding site of a single bond linking the first chemical moiety and the second chemical moiety.

In one embodiment of the invention, first chemical moiety comprises or consists of a structure of Formula Iaaaa:



Formula Iaaaa

wherein R^1, R^2, R^I and R^{Tz} are defined as above;
and R^D is the binding site of a single bond linking the first chemical moiety to the second chemical moiety.

In one embodiment, R^1, R^2 and R^I is at each occurrence independently from another selected from the group consisting of hydrogen (H), methyl, mesityl, tolyl and phenyl. The term tolyl comprises 2-tolyl, 3-tolyl and 4-tolyl.

In one embodiment, R^1, R^2 and R^I is at each occurrence independently from another selected from the group consisting of hydrogen (H), methyl, and phenyl.

In one embodiment, R^1, R^2, and R^I is at each occurrence independently from another selected from the group consisting of hydrogen (H), methyl, and phenyl.

In one embodiment, R^1, R^2 and R^I is at each occurrence hydrogen (H).

In one embodiment, R^V is R^A.

In one embodiment, R^W is R^A.

In one embodiment, R^T is R^A.

In one embodiment, R^X is R^A.

In one embodiment, R^Y is R^A.

In one embodiment, L^V is N.

In one embodiment, L^W is N.

In one embodiment, L^T is N.

In one embodiment, R^V is R^A, and L^V is N.

In one embodiment, R^V is R^A, and L^W is N.

In one embodiment, R^V is R^A, and L^T is N.

In one embodiment, R^W is R^A, and L^W is N.

In one embodiment, R^W is R^A, and L^T is N.

In one embodiment, R^W is R^A, and L^V is N.

In one embodiment, R^T is R^A, and L^W is N.

In one embodiment, R^T is R^A, and L^T is N.

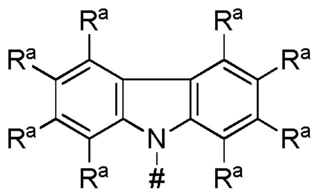
In one embodiment, R^T is R^A, and L^V is N.

In a further embodiment of the invention R^{Tz} is independently from each other selected from the group consisting of H, methyl,
phenyl, which is optionally substituted with one or more substituents R^6;
1,3,5-triazinyl, which is optionally substituted with one or more substituents R^6; and
pyrimidinyl, which is optionally substituted with one or more substituents R^6.

In a further embodiment of the invention, each of R^{Tz} is independently from each other selected from the group consisting of H, methyl and phenyl.

In a further embodiment of the invention, R^{Tz} is phenyl at each occurrence.

In a further embodiment of the invention, the second chemical moiety comprises or consists of a structure of Formula IIa:



Formula IIa

wherein # and R^a are defined as above.

In a further embodiment of the invention, R^a is at each occurrence independently from another selected from the group consisting of H,
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^a is at each occurrence independently from another selected from the group consisting of H,
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.

In a further embodiment of the invention, R^a is at each occurrence independently from another selected from the group consisting of H,

Me,

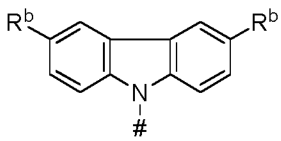
^{t}Bu,

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

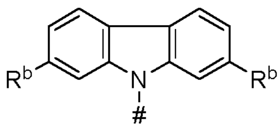
triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph.

In a further embodiment of the invention, R^a is H at each occurrence

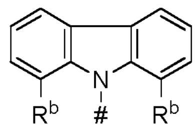
In a further embodiment of the invention, the second chemical moiety comprises or consists of a structure of Formula IIb, a structure of Formula IIb-2, a structure of Formula IIb-3 or a structure of Formula IIb-4:



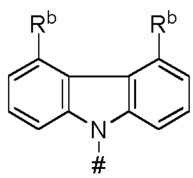
Formula IIb



Formula IIb-2



Formula IIb-3



Formula IIb-4

wherein

R^b is at each occurrence independently from another selected from the group consisting of

deuterium,

$N(R^5)_2$,

OR^5,

$Si(R^5)_3$,

$B(OR^5)_2$,

OSO_2R^5,

CF_3,

CN,

F,

Br,

I,

C_1-C_{40}-alkyl,

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

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

C_1-C_{40}-alkoxy,

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

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

C_1-C_{40}-thioalkoxy,

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

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

C_2-C_{40}-alkenyl,

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

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

C_2-C_{40}-alkynyl,

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

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

C_6-C_{60}-aryl,

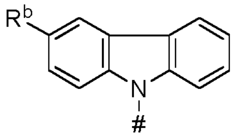
which is optionally substituted with one or more substituents R^5; and

C_3-C_{57}-heteroaryl,

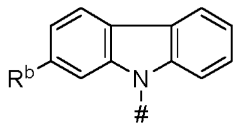
which is optionally substituted with one or more substituents R^5.

Apart from that the aforementioned definitions apply.

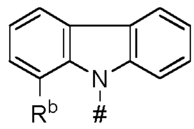
In one additional embodiment of the invention, the second chemical moiety comprises or consists of a structure of Formula IIc, a structure of Formula IIc-2, a structure of Formula IIc-3 or a structure of Formula IIc-4:



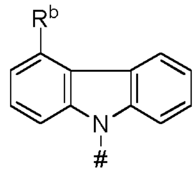
Formula IIc



Formula IIc-2



Formula IIc-3



Formula IIc-4

wherein the aforementioned definitions apply.

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

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,

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^b is at each occurrence independently from another selected from the group consisting of

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.

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

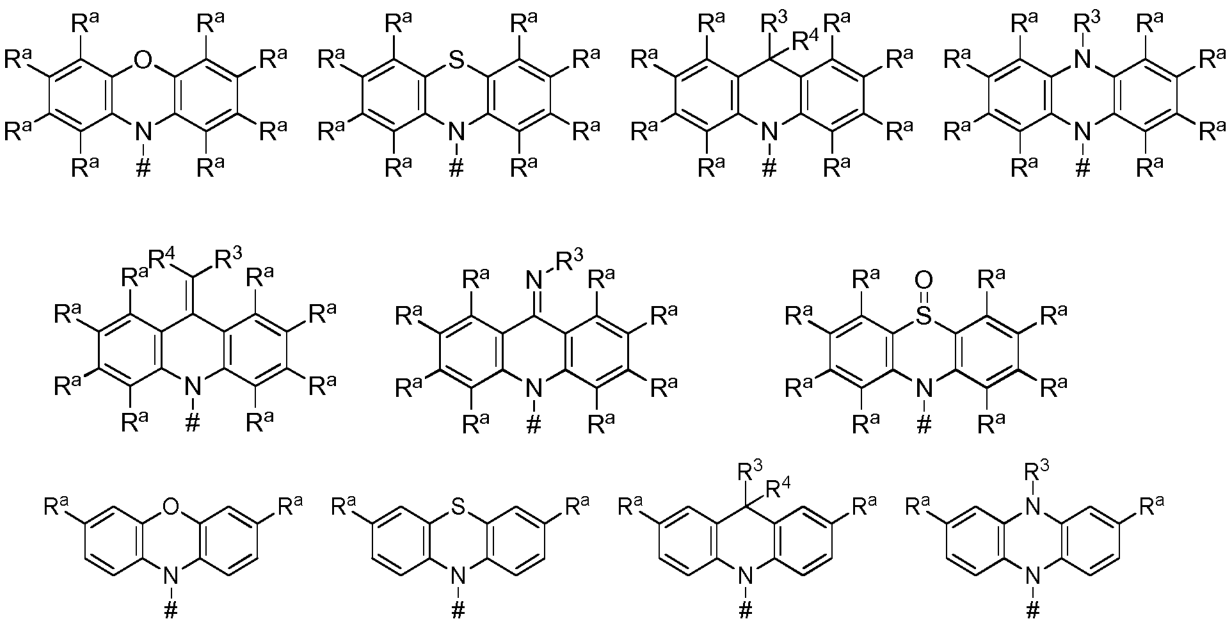
Me,

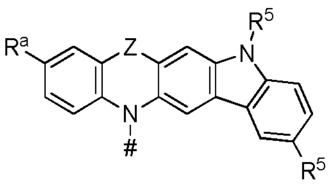
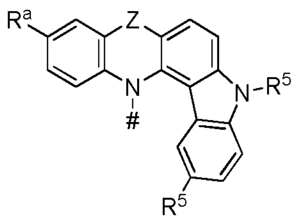
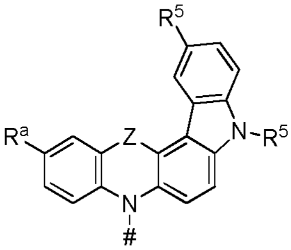
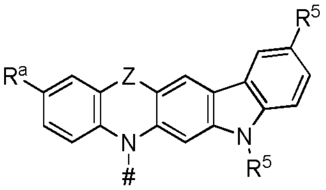
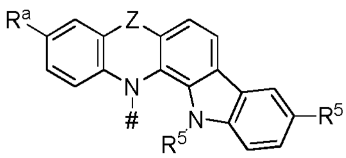
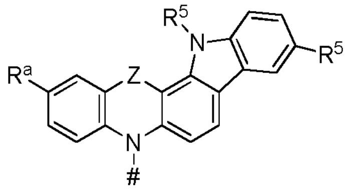
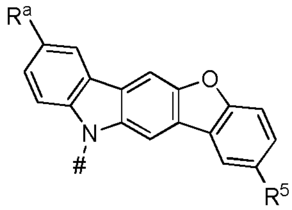
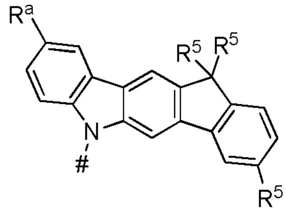
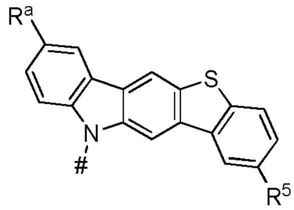
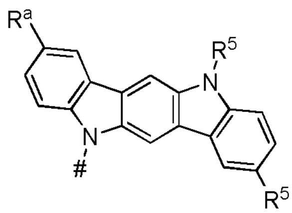
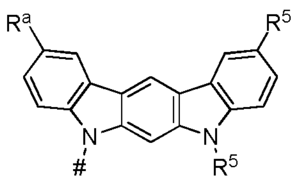
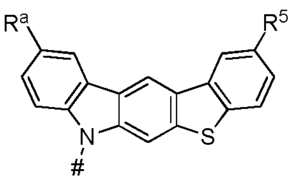
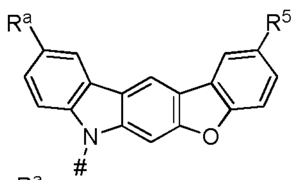
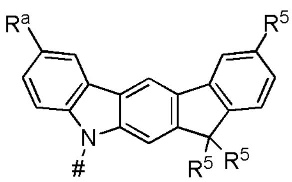
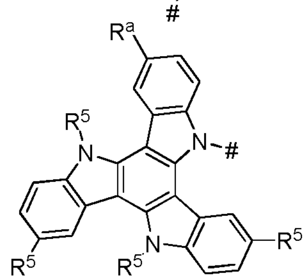
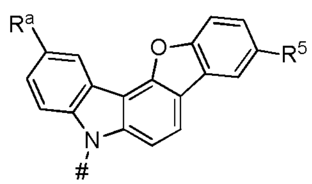
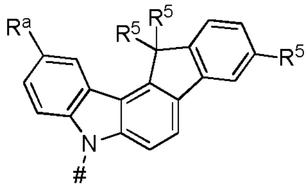
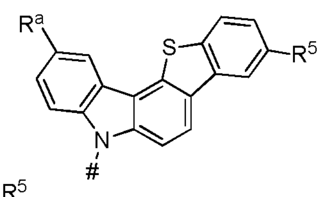
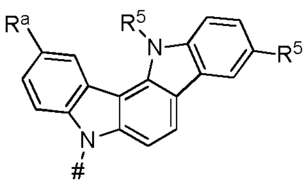
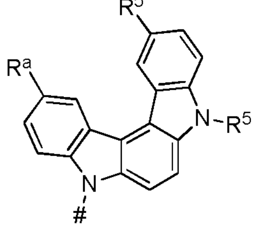
^{t}Bu,

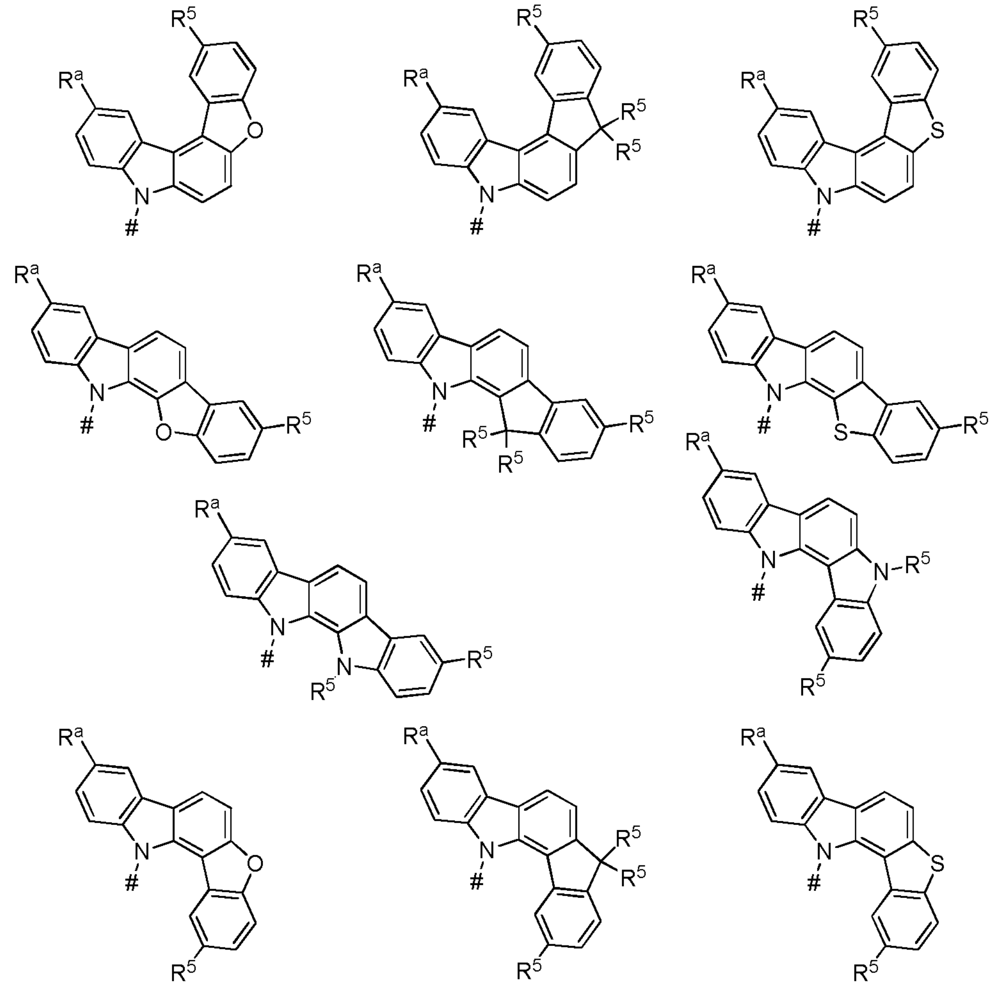
Ph, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

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.

In the following, exemplary embodiments of the second chemical moiety are shown:



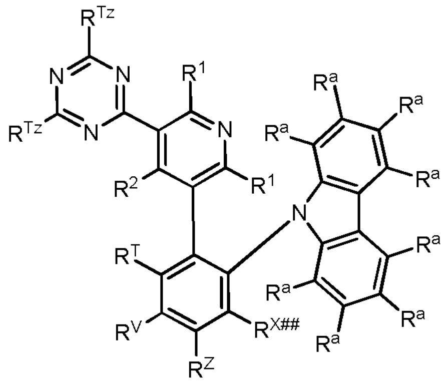























wherein for #, Z, R^a, R^3, R^4 and R^5 the aforementioned definitions apply.

In one embodiment, R^a and R^5 is at each occurrence independently from another selected from the group consisting of hydrogen (H), methyl (Me), i-propyl ($CH(CH_3)_2$) (^{i}Pr), t-butyl (^{t}Bu), phenyl (Ph), CN, CF_3, and diphenylamine (NPh_2).

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula III:



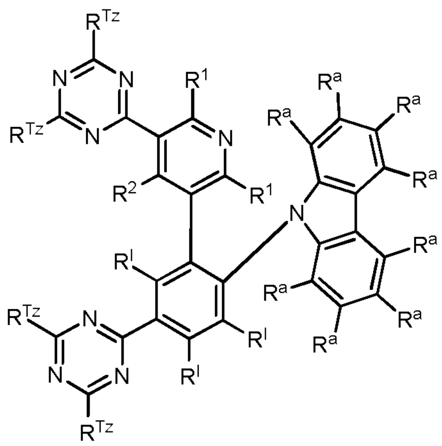
Formula III

wherein R^Z is selected from the group consisting of R^I and R^A,

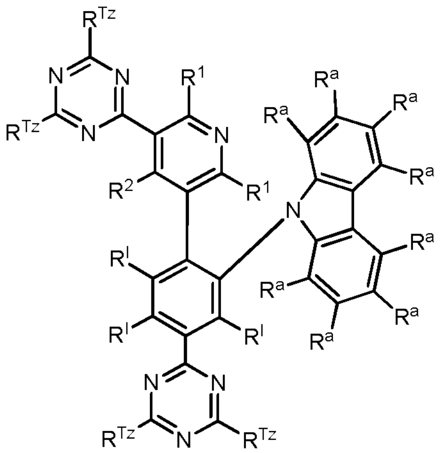
wherein $R^{X\#\#}$ is selected from the group consisting of R^I and R^A,
wherein exactly one substituent selected from the group consisting of R^V, R^T, $R^{X\#\#}$ and R^Z is R^A, and apart from that the aforementioned definitions apply.

In a preferred embodiment of the invention, the organic molecules comprise or consist of a structure of Formula III and R^V is R^A.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula III-1 and Formula III-2:



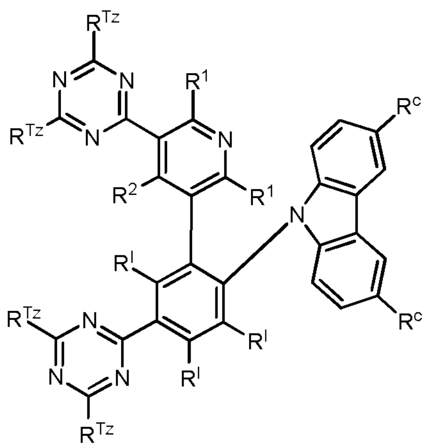
Formula III-1



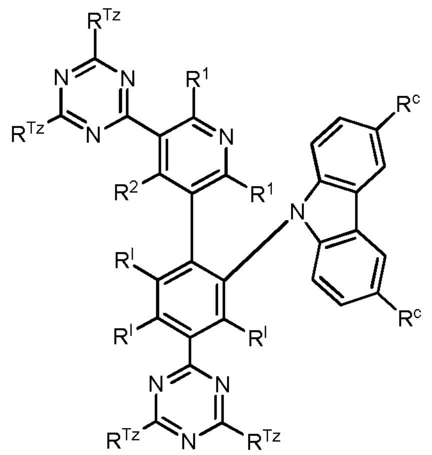
Formula III-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula IIIa-1 and Formula IIIa-2:



Formula IIIa-1



Formula IIIa-2

wherein

R^c is at each occurrence independently from another selected from the group consisting of

Me,

^iPr,

^{t}Bu,

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

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,

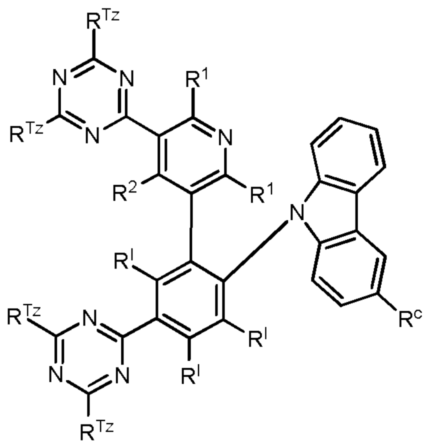
pyrimidinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

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,

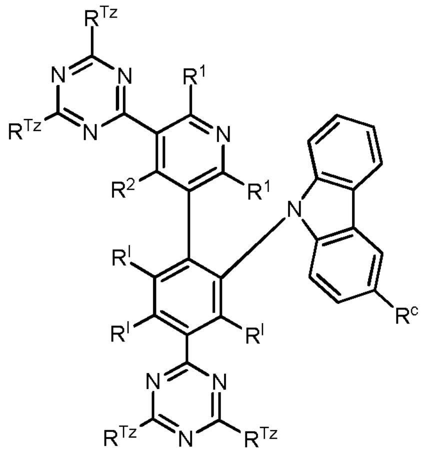
triazinyl, which is optionally substituted with one or more substituents independently from each other selected from the group consisting of Me, ^{i}Pr, ^{t}Bu, CN, CF_3, and Ph,

and $N(Ph)_2$.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula IIIb-1 and Formula IIIb-2:



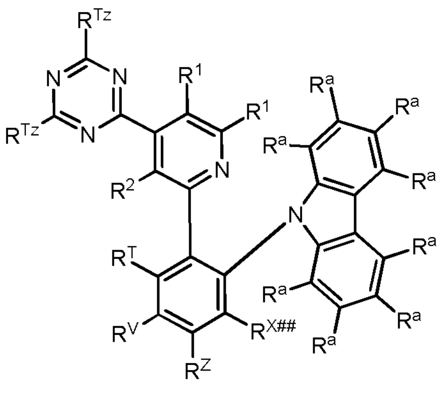
Formula IIIb-1



Formula IIIb-2

wherein the aforementioned definitions apply.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula IV:

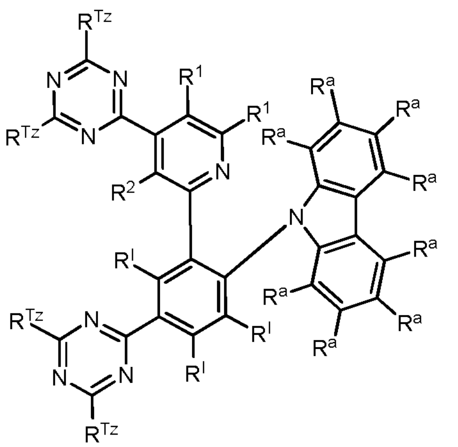


Formula IV

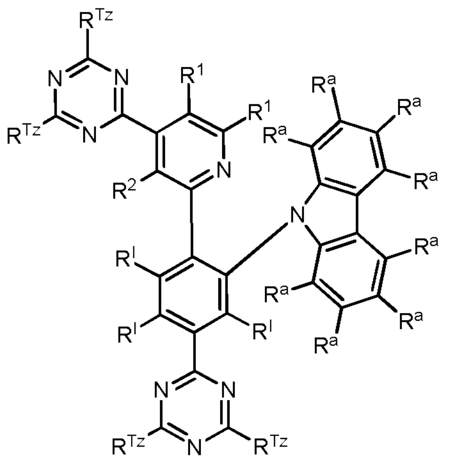
wherein the aforementioned definitions.

In a preferred embodiment of the invention, the organic molecules comprise or consist of a structure of Formula IV and R^V is R^A.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula IV-1 and Formula IV-2:



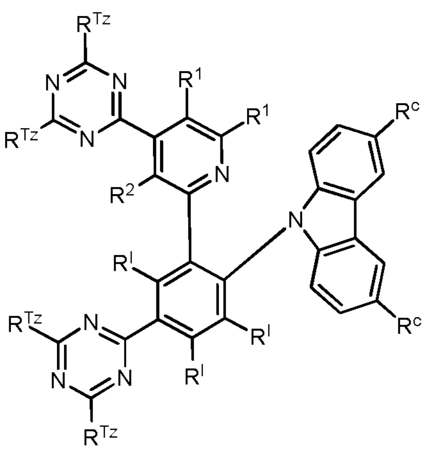
Formula IV-1



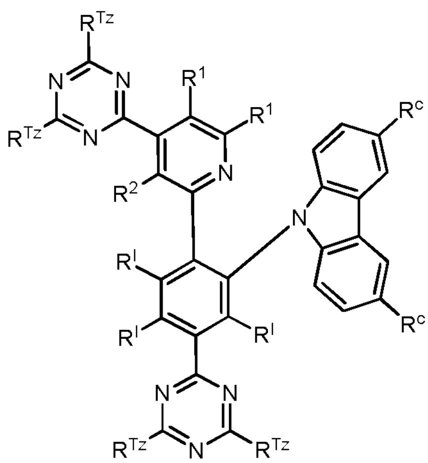
Formula IV-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula IVa-1 and Formula IVa-2:



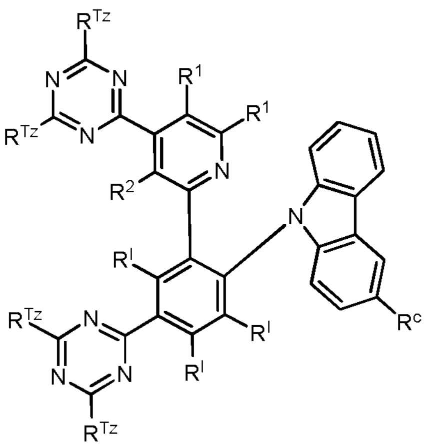
Formula IVa-1

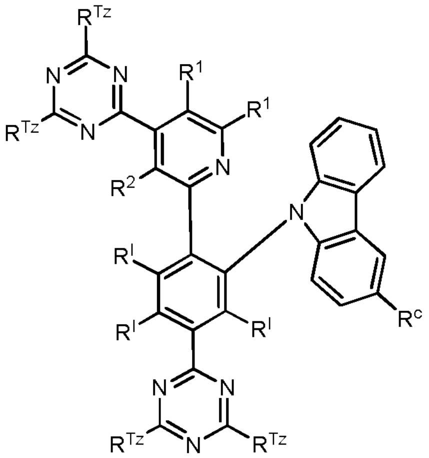


Formula IVa-2

wherein the aforementioned definitions apply.

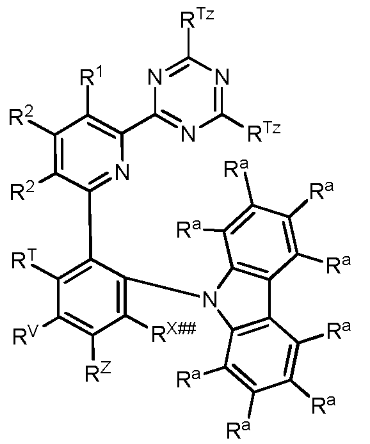
In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula IVb-1 and Formula IVb-2:


Formula IVb-1


Formula IVb-2

wherein the aforementioned definitions apply.

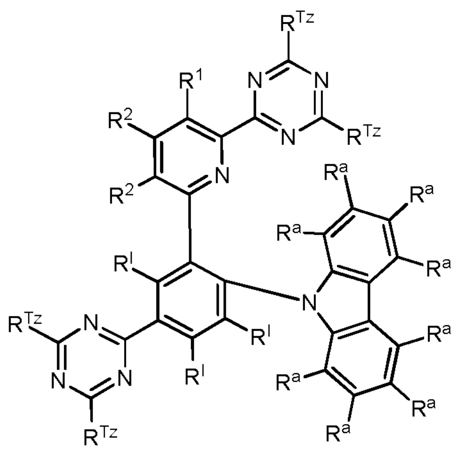
In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula V:


Formula V

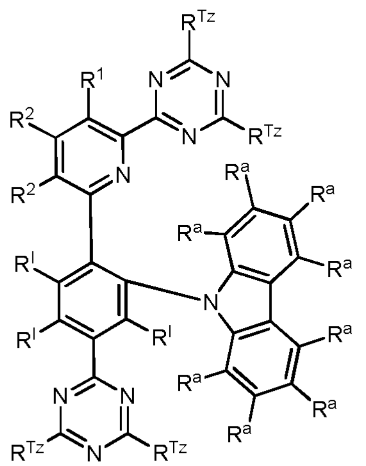
wherein the aforementioned definitions apply.

In a preferred embodiment of the invention, the organic molecules comprise or consist of a structure of Formula V and R^V is R^A.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula V-1 and Formula V-2:



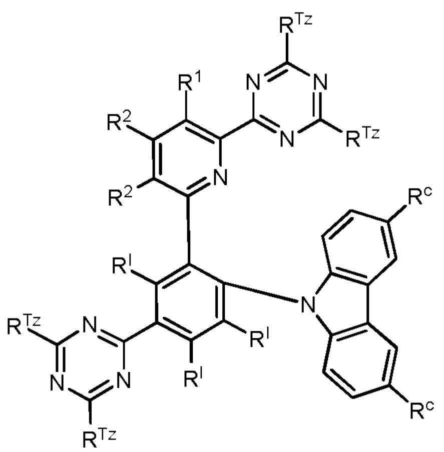
Formula V-1



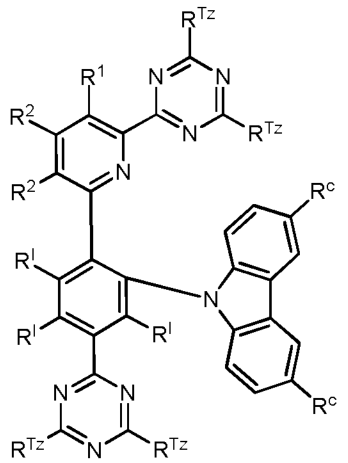
Formula V-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula Va-1 and Formula Va-2:



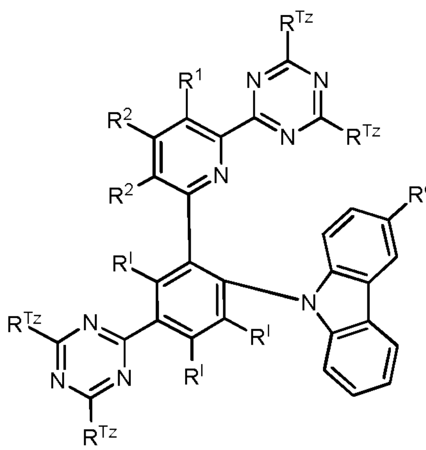
Formula Va-1



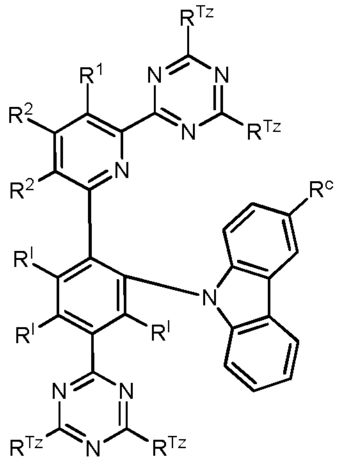
Formula Va-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula Vb-1 and Formula Vb-2:



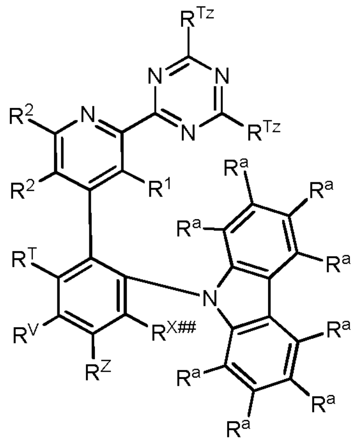
Formula Vb-1



Formula Vb-2

wherein the aforementioned definitions apply.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula VI:

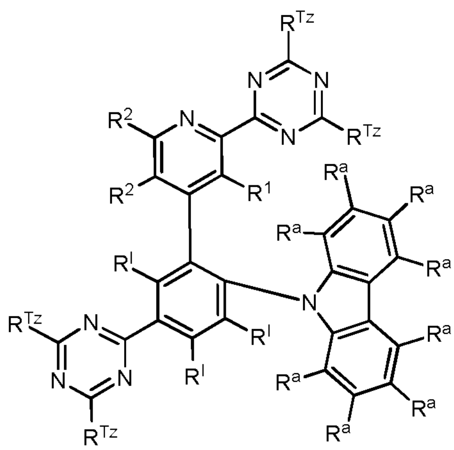


Formula VI

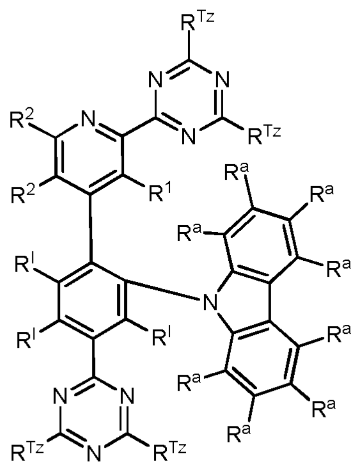
wherein the aforementioned definitions apply and wherein exactly one substituent selected from the group consisting of R^T, R^V, $R^{X\#\#}$ and R^Z is R^A.

In a preferred embodiment of the invention, the organic molecules comprise or consist of a structure of Formula VI and R^V is R^A.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VI-1 and Formula VI-2:



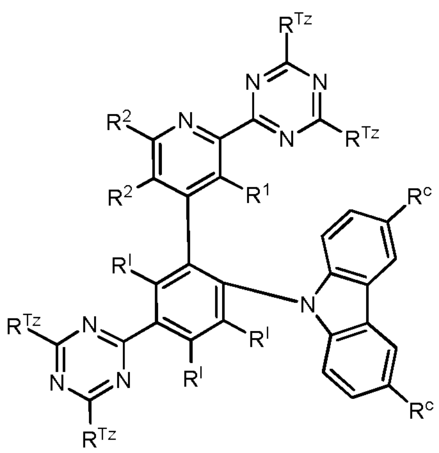
Formula VI-1



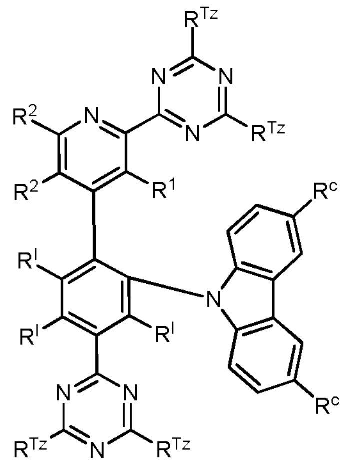
Formula VI-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIa-1 and Formula VIa-2:



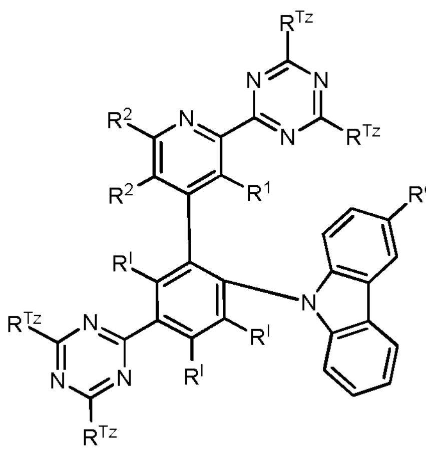
Formula VIa-1



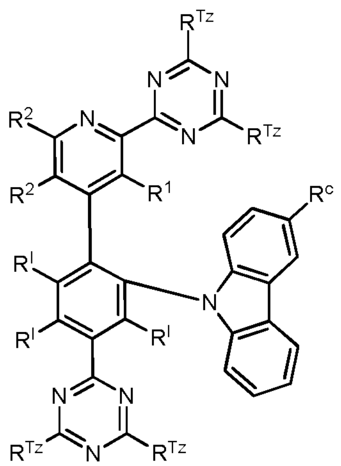
Formula VIa-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIb-1 and Formula VIb-2:



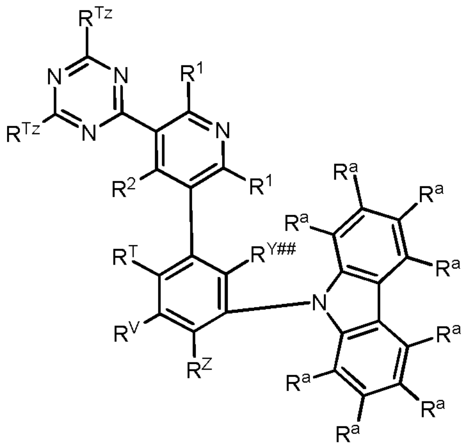
Formula VIb-1



Formula VIb-2

wherein the aforementioned definitions apply.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula VII:

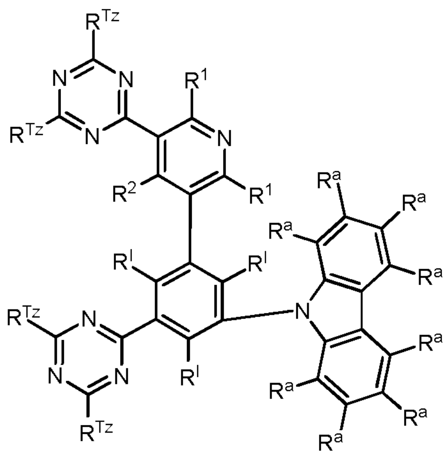


Formula VII

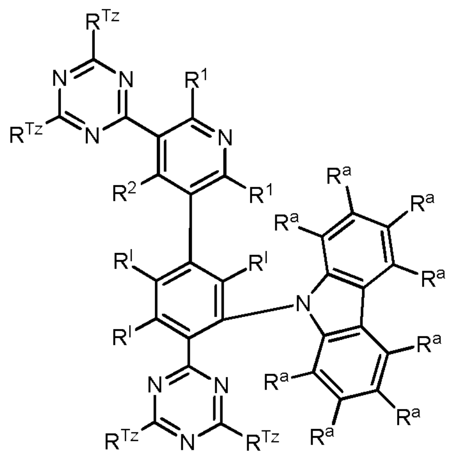
wherein the aforementioned definitions apply,
wherein $R^{Y\#\#}$ is selected from the group consisting of R^{I} and R^{A},
and wherein exactly one substituent selected from the group consisting of R^{V}, R^{T}, $R^{Y\#\#}$ and R^{Z} is R^{A}.

In another embodiment of the invention, the organic molecules comprise or consist of a structure of Formula VII and R^{V} is R^{A}.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VII-1 and Formula VII-2:



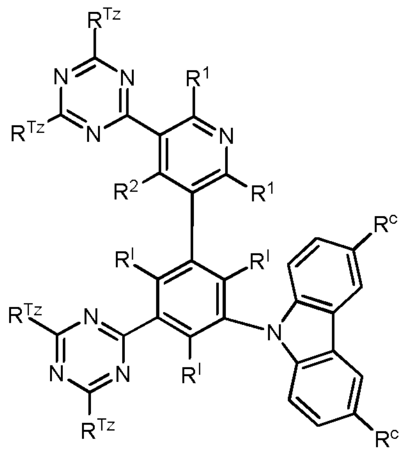
Formula VII-1



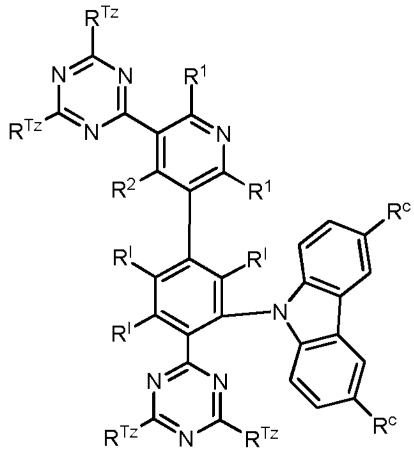
Formula VII-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIIa-1 and Formula VIIa-2:



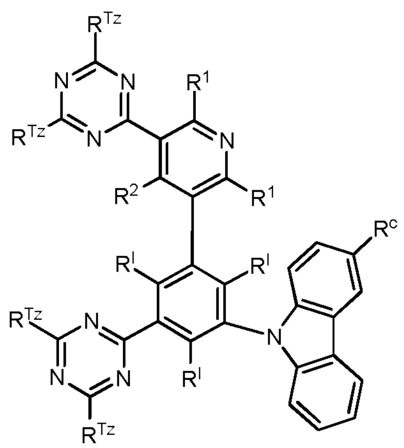
Formula VIIa-1

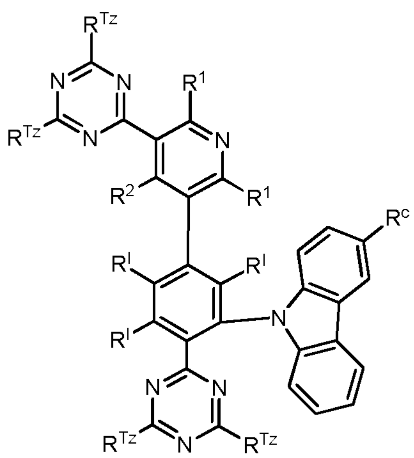


Formula VIIa-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIIb-1 and Formula VIIb-2:

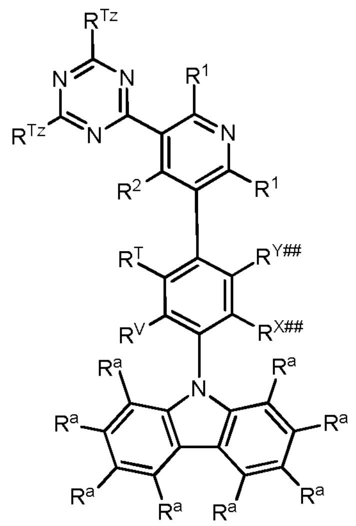




Formula VIIb-1 Formula VIIb-2

wherein the aforementioned definitions apply.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula VIII:

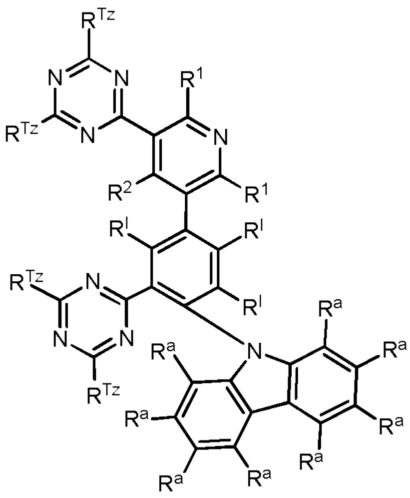


Formula VIII

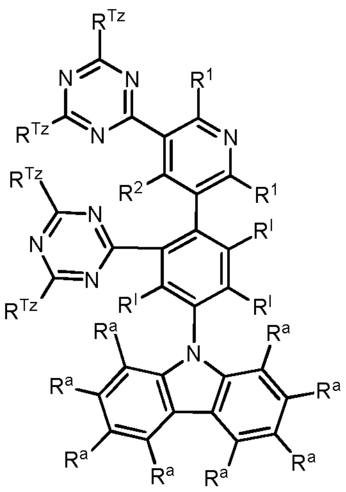
wherein the aforementioned definitions apply,
and wherein exactly one substituent selected from the group consisting of R^V, R^T, $R^{Y\#\#}$ and $R^{X\#\#}$ is R^A.

In another embodiment of the invention, the organic molecules comprise or consist of a structure of Formula VIII and R^V is R^A.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIII-1 and Formula VIII-2:



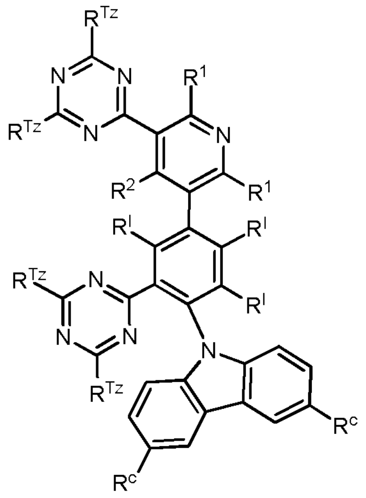
Formula VIII-1



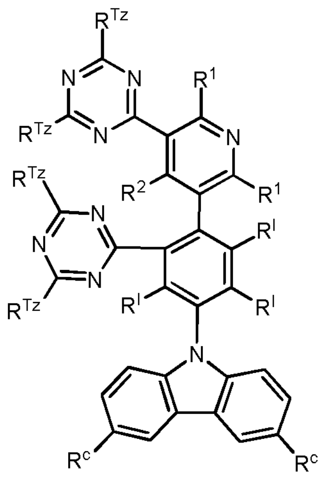
Formula VIII-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIIIa-1 and Formula VIIIa-2:



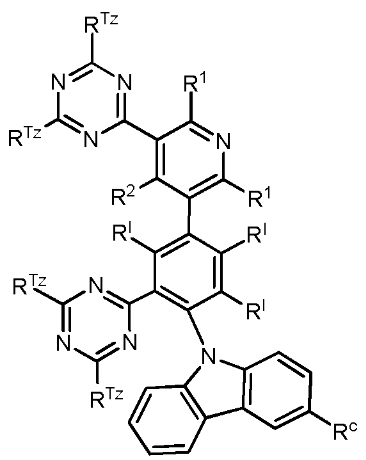
Formula VIIIa-1



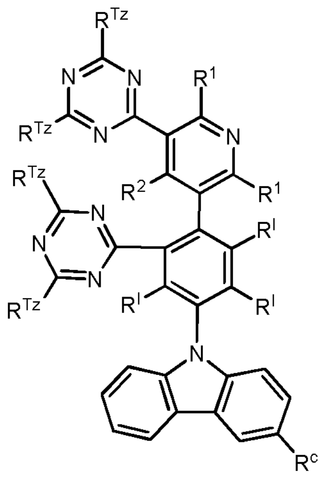
Formula VIIIa-2

wherein the aforementioned definitions apply.

In a further embodiment of the invention, the organic molecules comprise or consist of a structure selected from the group of Formula VIIIb-1 and Formula VIIIb-2:



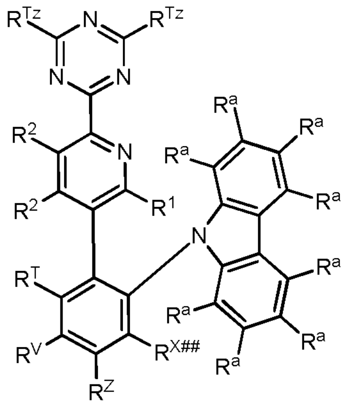
Formula VIIIb-1



Formula VIIIb-2

wherein the aforementioned definitions apply.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula IX:

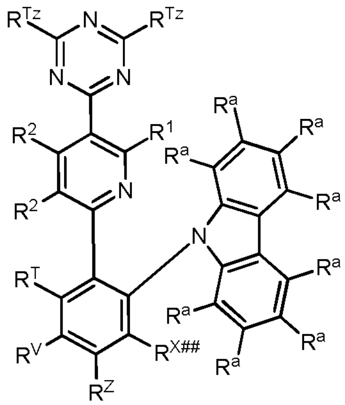


Formula IX

wherein the aforementioned definitions apply and wherein exactly one substituent selected from the group consisting of R^V, R^T, $R^{X\#\#}$ and R^Z is R^A.

In another embodiment of the invention, the organic molecules comprise or consist of a structure of Formula IX and R^V is R^A.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula X:

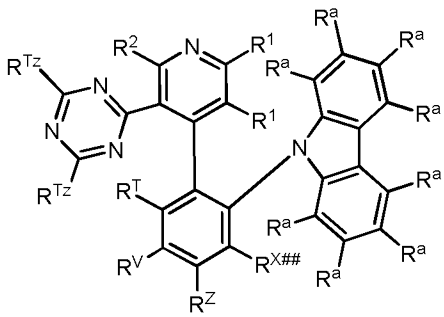


Formula X

wherein the aforementioned definitions apply and wherein exactly one substituent selected from the group consisting of R^V, R^T, $R^{X\#\#}$ and R^Z is R^A.

In another embodiment of the invention, the organic molecules comprise or consist of a structure of Formula X and R^V is R^A.

In one embodiment of the invention, the organic molecules comprise or consist of a structure of Formula XI:



Formula XI

wherein the aforementioned definitions apply and wherein exactly one substituent selected from the group consisting of R^V, R^T, $R^{X\#\#}$ and R^Z is R^A.

In another embodiment of the invention, the organic molecules comprise or consist of a structure of Formula XI and R^V is R^A.

In one embodiment of the invention R^c is at each occurrence independently from another selected from the group consisting of

Me,

^{i}Pr,

^{t}Bu,

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

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 one embodiment of the invention, the organic molecules according to the invention represent thermally-activated delayed fluorescence (TADF) emitters, which 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 5000 cm^{-1}, preferably 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 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 0.50 eV, preferably less than 0.48 eV, more preferably less than 0.45 eV, even more preferably less than 0.43 eV or even less than 0.40 eV in a film of poly(methyl methacrylate) (PMMA) with 10 % by weight of organic molecule at room temperature.

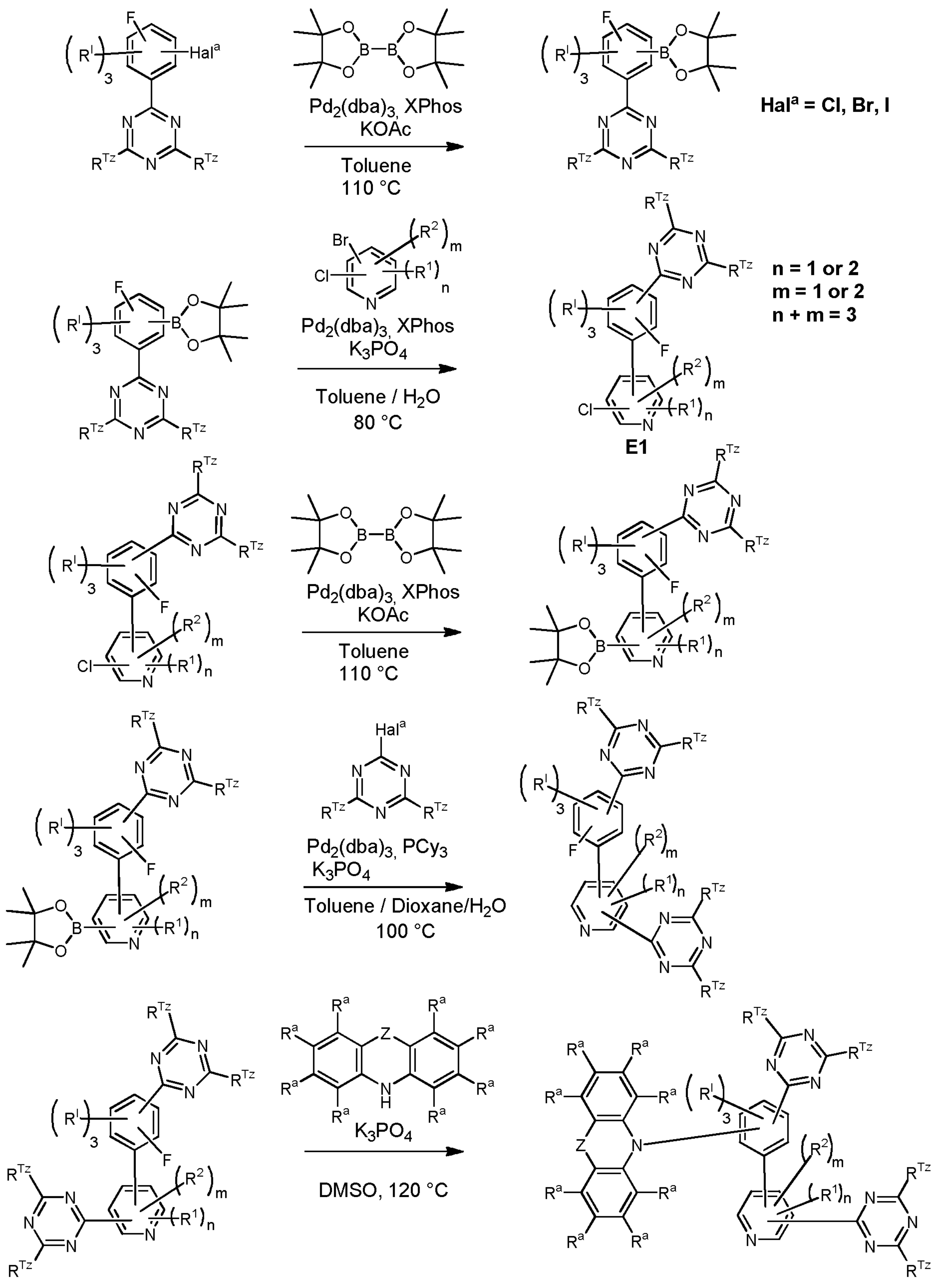
In a further embodiment of the invention, the organic molecules according to the invention have a “blue material index” (BMI), calculated by dividing the photoluminescence quantum yield (PLQY) in % by the CIEy color coordinate of the emitted light, of more than 150, in particular more than 200, preferably more than 250, more preferably of more than 300 or even more than 500.

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 organic molecules (with an optional subsequent reaction) according to the invention, wherein a halo-fluorophenyl-1,3,5-triazine, in which the central phenyl ring is substituted with three R^{I}-substituents and the triazine unit is substituted with two R^{Tz} in 4- and 6-position, is used as a reactant:



Preferably, Hal^a-fluorophenyl-1,3,5-triazine is selected from bromo-fluorophenyl-1,3,5-triazines and chloro-fluorophenyl-1,3,5-triazines. Exemplary Hal^a-fluorophenyl-1,3,5-triazines are 2-(3-Bromo-4-fluorophenyl)-4,6-diphenyl-1,3,5-triazine, 2-(3-Chloro-4-fluorophenyl)-4,6-diphenyl-1,3,5-triazine, 2-(3-Bromo-4-fluorophenyl)-4,6-methyl-1,3,5-triazine, 2-(3-Chloro-4-

fluorophenyl)-4,6-methyl-1,3,5-triazine, 2-(4-Bromo-3-fluorophenyl)-4,6-diphenyl-1,3,5-triazine, 2-(4-Chloro-3-fluorophenyl)-4,6-diphenyl-1,3,5-triazine, 2-(4-Bromo-3-fluorophenyl)-4,6-methyl-1,3,5-triazine, 2-(4-Chloro-3-fluorophenyl)-4,6-methyl-1,3,5-triazine.
Preferably, the Hal^a-fluoro-pyridine reactant is selected from chloro-fluoropyridine and bromo-fluoropyridine. Exemplary Hal^a-fluoro-pyridines are 4-chloro-3-fluoro-pyridine, 4-chloro-2-fluoro-pyridine, 3-chloro-4-fluoro-pyridine, 3-chloro-5-fluoro-pyridine, 3-chloro-6-fluoro-pyridine, 3-chloro-2-fluoro-pyridine, 2-chloro-3-fluoro-pyridine, 2-chloro-4-fluoro-pyridine, 2-chloro-5-fluoro-pyridine, 2-chloro-6-fluoro-pyridine, 3-bromo-4-fluoro-pyridine, 3-bromo-5-fluoro-pyridine, 3-bromo-6-fluoro-pyridine, 3-bromo-2-fluoro-pyridine, 2-bromo-3-fluoro-pyridine, 2-bromo-4-fluoro-pyridine, 2-bromo-5-fluoro-pyridine and 2-bromo-6-fluoro-pyridine, which are each substituted with either one R^1 and two R^2 or two R^1 and one R^2 at the remaining positions.

Typically, $Pd_2(dba)_3$ (tris(dibenzylideneacetone)dipalladium(0)) is used as a Pd catalyst, but alternatives are known in the art. For example, the ligand may be selected from the group consisting of S-Phos ([2-dicyclohexylphoshino-2',6'-dimethoxy-1,1'-biphenyl]; or SPhos), X-Phos (2-(dicyclohexylphosphino)-2'',4'',6''-triisopropylbiphenyl; or XPhos), and $P(Cy)_3$ (tricyclohexylphosphine). The salt is, for example, selected from tribasic potassium phosphate and potassium acetate and the solvent can be a pure solvent, such as toluene or dioxane, or a mixture, such as toluene/dioxane/water or dioxane/toluene. A person of skill in the art can determine which Pd catalyst, ligand, salt and solvent combination will result in high reaction yields.

A person of skill in the pertinent art is aware that instead of the *in-situ* generation of a boronic acid ester by reacting a halo-species with bis-(pinacolato)diboron and then reacting it with another halo-species as described here, alternative synthesis routes can be chosen. For example, one of the two halo-species, i.e. the Hal^a-fluorophenyl-1,3,5-triazine and the halo-fluoro-pyridine, can be replaced by the corresponding boronic acid or boronic acid ester species and reacted with the respective other halo-species in a typical cross-coupling reaction.

For the reaction of **E1** with a nitrogen heterocycle in a nucleophilic aromatic substitution with an aryl halide, preferably an aryl fluoride, typical conditions include the use of a base, such as tribasic potassium phosphate or sodium hydride, for example, in an aprotic polar solvent, such as dimethyl sulfoxide (DMSO) or N,N-dimethylformamide (DMF), for example.

An alternative synthesis route comprises the introduction of a nitrogen heterocycle via copper- or palladium-catalyzed coupling to an aryl halide or aryl pseudohalide, preferably an aryl bromide, an aryl iodide, aryl triflate or an aryl tosylate.

A further aspect of the invention relates to the use of an organic molecule according to the invention as a luminescent emitter or as an absorber, and/or as host material and/or as electron transport material, and/or as hole injection material, and/or as hole blocking material 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, the optoelectronic device may be able to emit light in the visible range, i.e., of from 400 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 vapour sensors not hermetically externally shielded,
- 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 optoelectronic 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 OLEDs, is 1 % to 99 % by weight, more particularly 5 % 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.

Particularly preferably 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 E;
(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 E, 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 E;

(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 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 optoelectronic 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.

Exemplarily, when the optoelectronic device is an OLED, it may exhibit 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 only optionally, different layers may be merged and the OLED may comprise more than one layer of each layer type defined above.

Furthermore, the optoelectronic device may optionally comprise one or more protective layers protecting the device from damaging exposure to harmful species in the environment including, exemplarily moisture, vapor and/or gases.

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

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

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

Particularly preferably, the anode layer A (essentially) consists 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) typically a hole transport layer (HTL) is located. Herein, any hole transport compound may be used. Exemplarily, 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. Exemplarily 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), typically, the light-emitting layer EML is 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 E. 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 molecule according to the invention E 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 exemplarily 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. Exemplarily, the cathode layer C may comprise or may consist of a metal (e.g., Al, Au, Ag, Pt, Cu, Zn, Ni, Fe, Pb, LiF, Ca, Ba, Mg, In, W, or Pd) or a metal alloy. For practical reasons, the cathode layer may also consist of (essentially) non-transparent metals such as Mg, Ca or Al. Alternatively or additionally, the cathode layer C may also comprise graphite and or carbon nanotubes (CNTs). Alternatively, the cathode layer C may also 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, also the electron transport layer (ETL) and/or a hole blocking layer (HBL) may 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 emitter molecule according to the invention E 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 emitter molecule E. 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 optoelectronic device (e.g., an OLED) may exemplarily be an essentially white optoelectronic device. Exemplarily such white optoelectronic device may comprise at least one (deep) blue emitter molecule and one or more emitter molecules emitting green and/or red light. Then, there may also optionally be energy transmittance between two or more molecules as described above.

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 0.50 eV, preferably less than 0.48 eV, more preferably less than 0.45 eV, even more preferably less than 0.43 eV or even less than 0.40 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 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 optoelectronic device, in particular the OLED according to the present invention can be produced by any means of vapor deposition and/ or liquid processing. Accordingly, at least one layer is

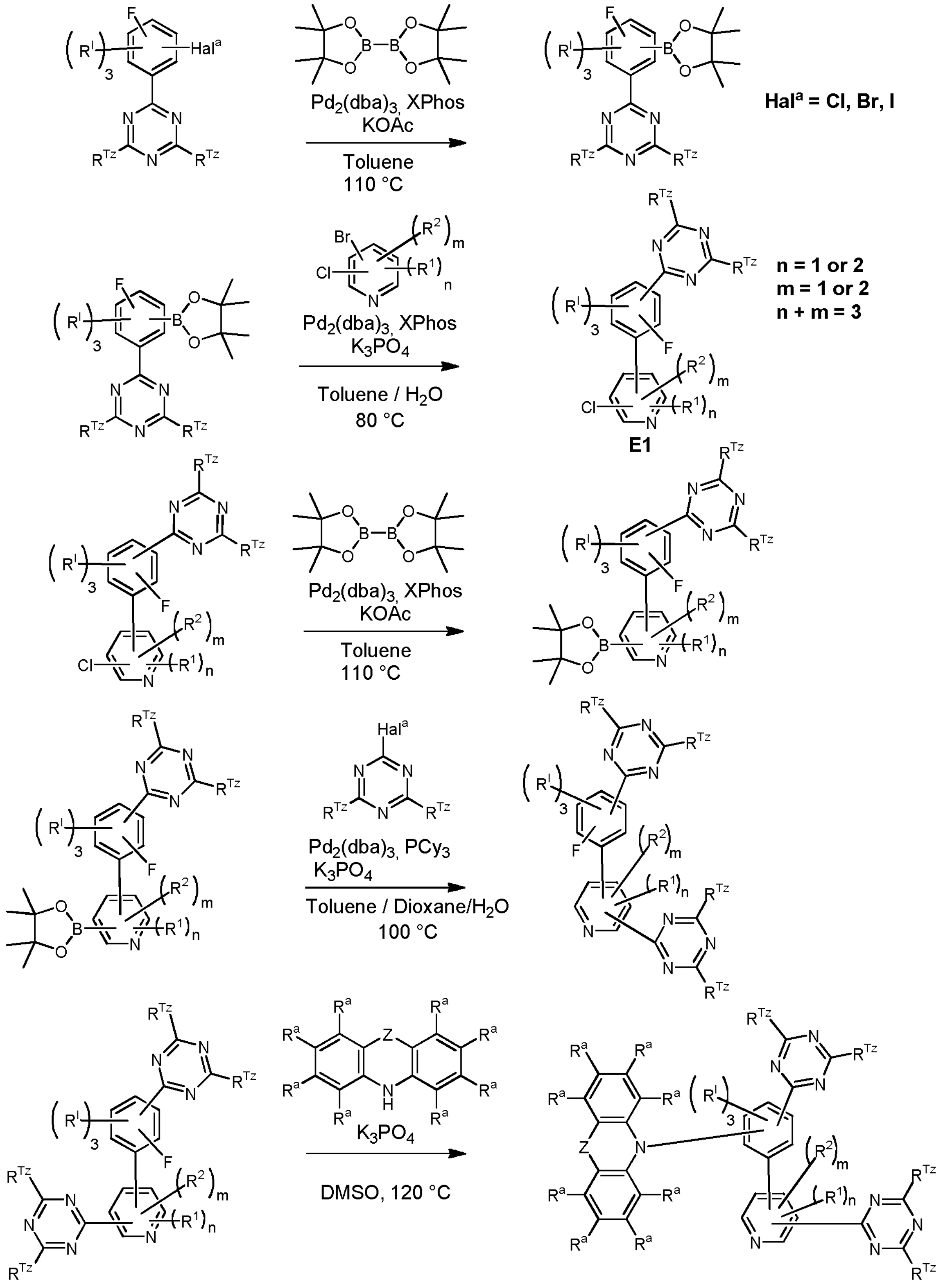
- prepared by means of a sublimation process,
- prepared by means of an organic vapor phase deposition process,
- prepared by means of a carrier gas sublimation process,
- solution processed or printed.

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

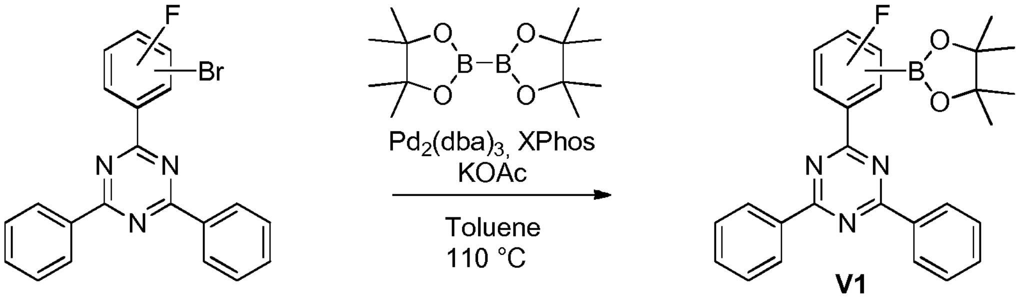
Vapor deposition processes exemplarily comprise thermal (co)evaporation, chemical vapor deposition and physical vapor deposition. For active matrix OLED display, an AMOLED backplane is used as substrate. The individual layer may be processed from solutions or dispersions employing adequate solvents. 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



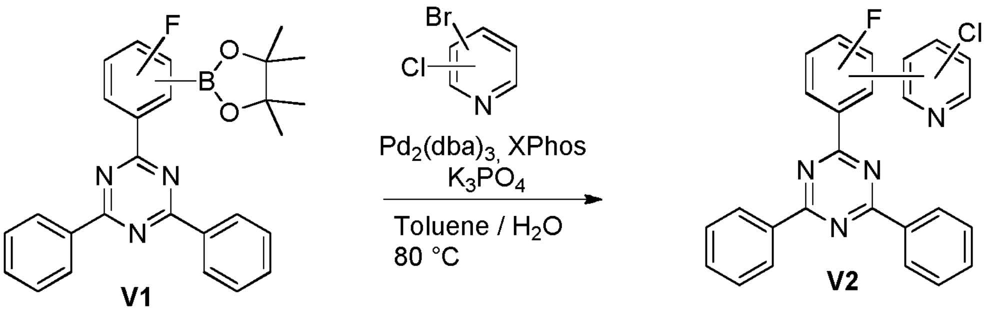
*General procedure for synthesis **AAV1***:



V1

2-(Bromo-fluorophenyl)-4,6-diphenyl-1,3,5-triazine (1.00 equivalent), bis-(pinacolato)diboron (1.5 equivalents, CAS: 73183-34-3), tris(dibenzylideneacetone)dipalladium(0) $Pd_2(dba)_3$ (0.04 equivalents, CAS: 51364-51-3), XPhos (0.08 equivalents, CAS 564483-18-7) and potassium acetate (KOAc, 3.0 equivalents) are stirred under nitrogen atmosphere in dry toluene at 110 °C for 16 h. After cooling down to room temperature (RT) the reaction mixture is extracted with ethyl acetate/brine. The organic phases are collected, washed with brine and dried over $MgSO_4$. The organic solvent is removed, the crude product was washed with cyclohexane and recrystallized from EtOH.

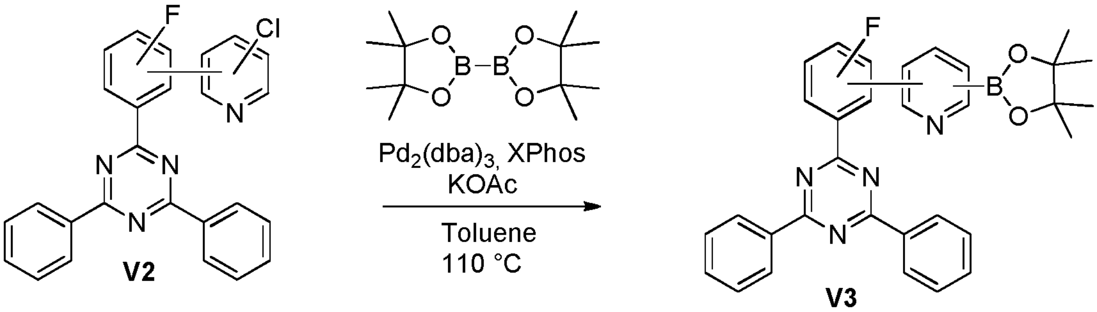
*General procedure for synthesis **AAV2***:



V1 **V2**

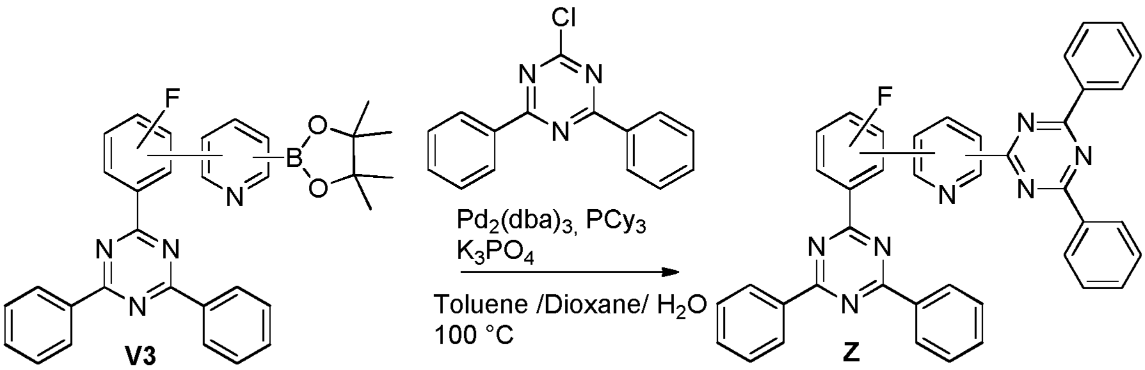
V1 (1.00 equivalent), bromo-chloro-pyridine (1.1 equivalents), tris(dibenzylideneacetone)dipalladium(0) $Pd_2(dba)_3$ (0.04 equivalents, CAS: 51364-51-3), X-Phos (0.08 equivalents, CAS 564483-18-7) and potassium phosphate (K_3PO_4, 3.0 equivalents) are stirred under nitrogen atmosphere in toluene/H_2O (6:1) at 80°C for 16 h. After cooling down to room temperature (RT) and the reaction mixture is poured onto water, solid is collected and washed with cyclohexane and dried under vacuum.

General procedure for synthesis ***AAV3***:



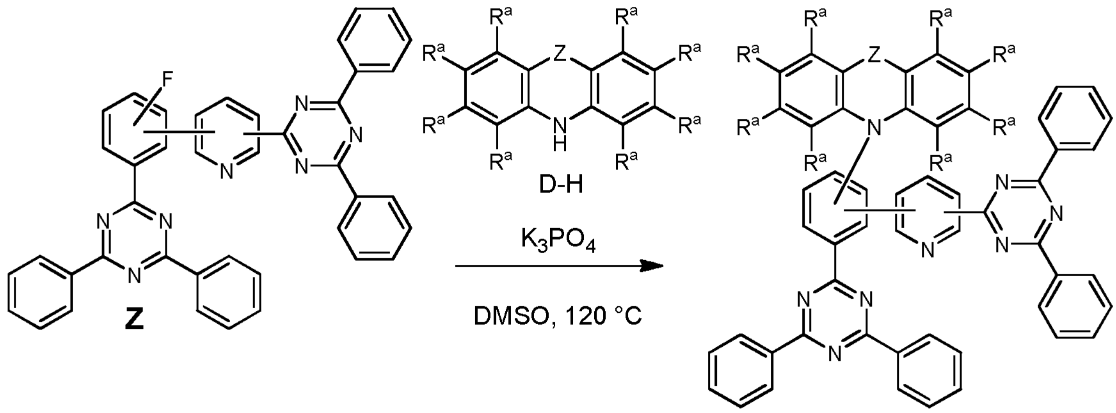
V2 (1.00 equivalent), bis-(pinacolato)diboron (1.5 equivalents, CAS: 73183-34-3), tris(dibenzylideneacetone)dipalladium(0) $Pd_2(dba)_3$ (0.04 equivalents, CAS: 51364-51-3), X-Phos (0.08 equivalents, CAS 564483-18-7) and potassium acetate (KOAc, 3.0 equivalents) are stirred under nitrogen atmosphere in dry toluene at 110 °C for 16 h. After cooling down to room temperature (RT) the reaction is poured onto water, filtrated and washed with water. The raw product is hardly soluble and used directly in the next step without further purification.

General procedure for synthesis ***AAV4***:



V3 (1.00 equivalent), 2-chloro-4,6-diphenyl-1,3,5-triazine (1.00 equivalent) (CAS: 3842-55-5), tricyclohexylphosphine 0.14 equivalents, CAS: 2622-14-2), tris(dibenzylideneacetone)dipalladium(0) $Pd_2(dba)_3$ (0.06 equivalents, CAS: 51364-51-3), and potassium phosphate (K_3PO_4, 3.0 equivalents) are stirred under nitrogen atmosphere in toluene/dioxane/H_2O (8:4:1) at 100 °C for 16 h. After cooling down to room temperature (RT) the reaction is poured into distilled water, filtrated and washed with water and cyclohexane. The raw product is hardly soluble and used directly in the next step without further purification.

General procedure for synthesis ***AAV5***:



Z (1.00 equivalent), corresponding donor molecule D-H (0.75-1.00 equivalents) and tribasic potassium phosphate (3.00 equivalents) are suspended under nitrogen atmosphere in dry DMSO and stirred at 120 °C (16 h). After cooling down to room temperature (RT) the reaction mixture is extracted with dichloroethane /brine. Organic phases are collected, washed with brine and dried over $MgSO_4$. The solvent is evaporated under reduced pressure. The crude product is purified by recrystallization or by flash chromatography.

In particular, the donor molecule D-H is a 3,6-substituted carbazole (e.g., 3,6-dimethylcarbazole, 3,6-diphenylcarbazole, 3,6-di-tert-butylcarbazole), a 2,7-substituted carbazole (e.g., 2,7-dimethylcarbazole, 2,7-diphenylcarbazole, 2,7-di-tert-butylcarbazole), a 1,8-substituted carbazole (e.g., 1,8-dimethylcarbazole, 1,8-diphenylcarbazole, 1,8-di-tert-butylcarbazole), a 1-substituted carbazole (e.g., 1-methylcarbazole, 1-phenylcarbazole, 1-tert-butylcarbazole), a 2-substituted carbazole (e.g., 2-methylcarbazole, 2-phenylcarbazole, 2-tert-butylcarbazole), or a 3-substituted carbazole (e.g., 3-methylcarbazole, 3-phenylcarbazole, 3-tert-butylcarbazole).

For example, a halogen-substituted carbazole, particularly 3-bromocarbazole, can be used as D-H.

In a subsequent reaction, a boronic acid ester functional group or boronic acid functional group may, for example, be introduced at the position of the one or more halogen substituents, which was introduced via D-H, to yield the corresponding carbazol-3-ylboronic acid ester or carbazol-3-ylboronic acid, e.g., via the reaction with bis(pinacolato)diboron (CAS No. 73183-34-3). Subsequently, one or more substituents R^a may be introduced in place of the boronic acid ester group or the boronic acid group via a coupling reaction with the corresponding halogenated reactant R^a-Hal, preferably R^a-Cl and R^a-Br.
Alternatively, one or more substituents R^a may be introduced at the position of the one or more halogen substituents, which was introduced via D-H, via the reaction with a boronic acid of the substituent R^a [R^a-$B(OH)_2$] or a corresponding boronic acid ester.

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 a saturated calomel electrode (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 dried 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:

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

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

Production and characterization of optoelectronic 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 %.

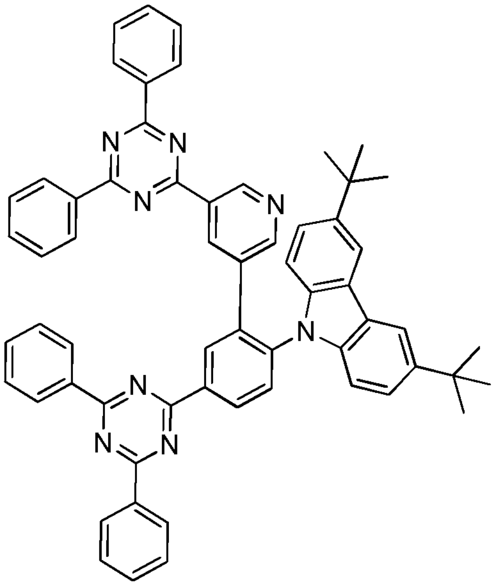
The not fully optimized OLEDs are characterized using standard methods and measuring electroluminescence spectra, the external quantum efficiency (in %) in dependency on the intensity, calculated using the light detected by the photodiode, and the current. The OLED device lifetime is extracted from the 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/m^2 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.

Example 1

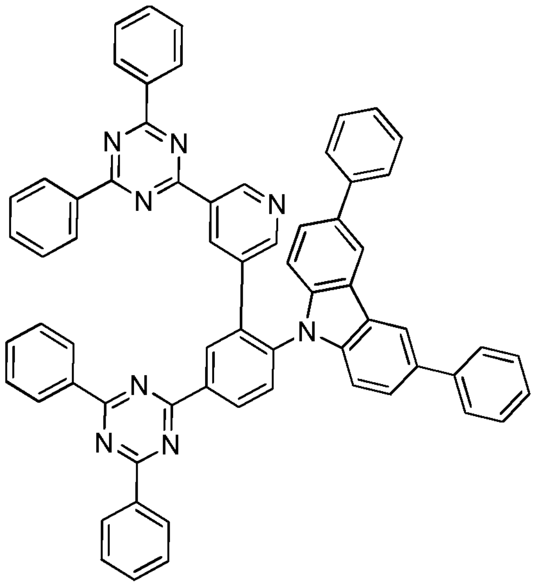


Example **1** was synthesized according to ***AAV1***, wherein 2-(4-fluoro-3-bromo-phenyl)-4,6-diphenyl-1,3,5-triazine was used as reactant (yield: 62%),
AAV2, wherein 3-bromo-5-chloropyridine (CAS 73583-39-8) was used as reactant (yield: 94%),
AAV3 (raw product used without further purification),
AAV4 (raw product used without further purification), wherein 2-chloro-4,6-diphenyl-1,3,5-triazine (CAS 3842-55-5) was used as reactant,
and ***AAV5*** , wherein 3,6-di-*tert*-butylcarbazole (CAS 37500-95-1) was used as reactant (28 % yield).

HPLC-MS: 28.45 min (894.52 m/z (100%))

Figure 1 depicts the emission spectrum of example **1** (10 % by weight in PMMA). The emission maximum (λ_{max}) is at 450 nm. The photoluminescence quantum yield (PLQY) is 56 %, the full width at half maximum (FWHM) is 0.41 eV. The resulting CIE_x coordinate is determined at 0.16 and the CIE_y coordinate at 0.14. The emission lifetime is 30 µs.

Example 2

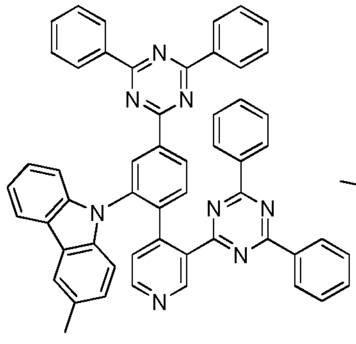
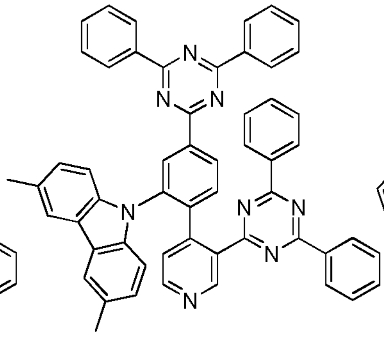
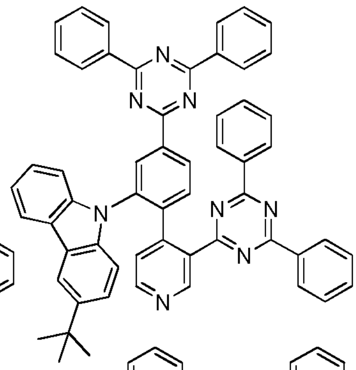
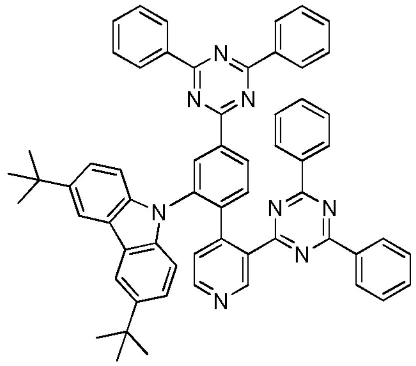
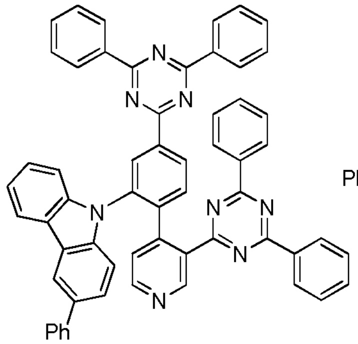
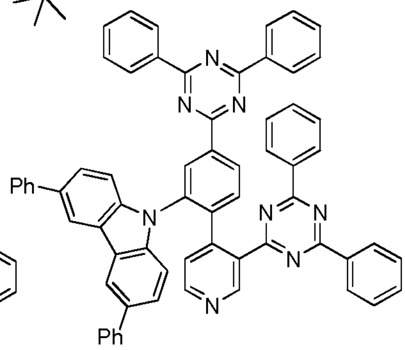
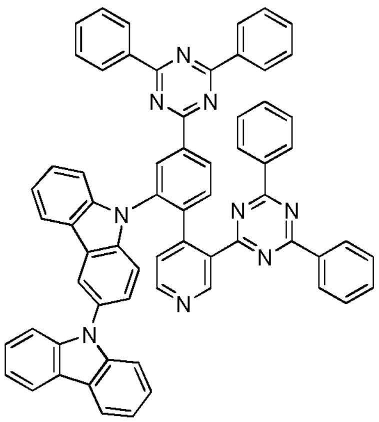
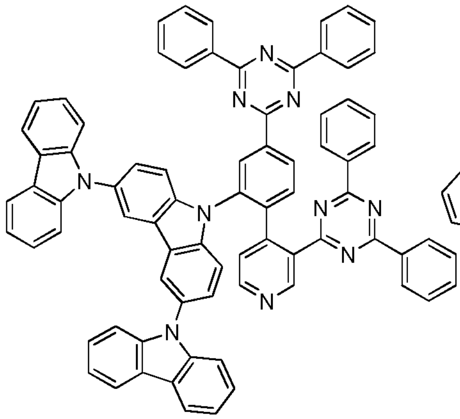
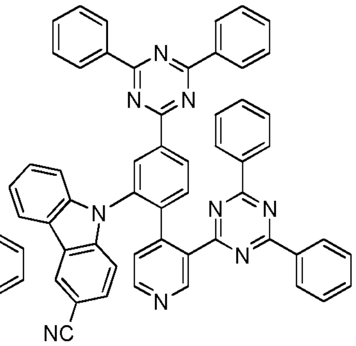
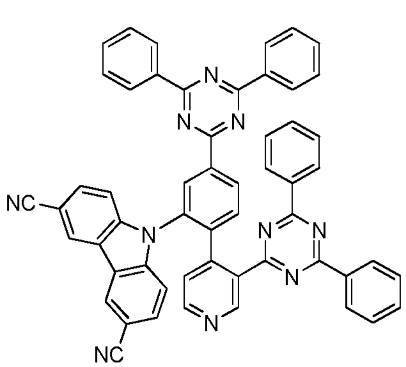
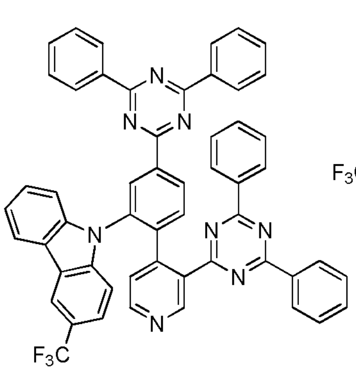
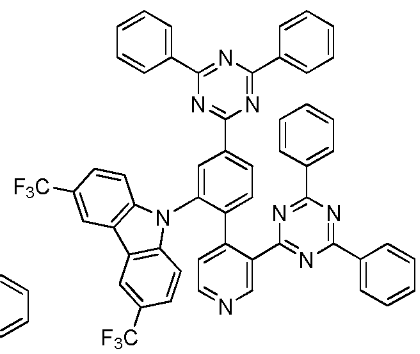


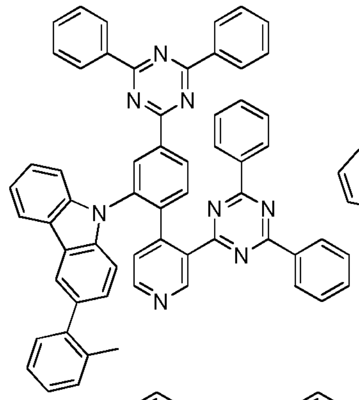
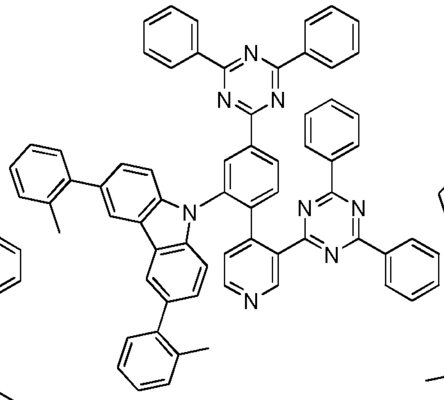
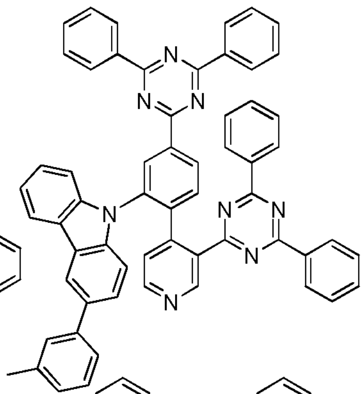
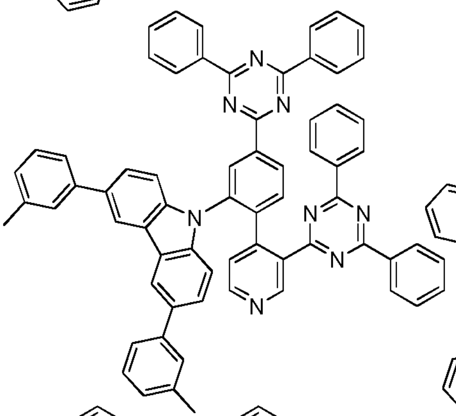
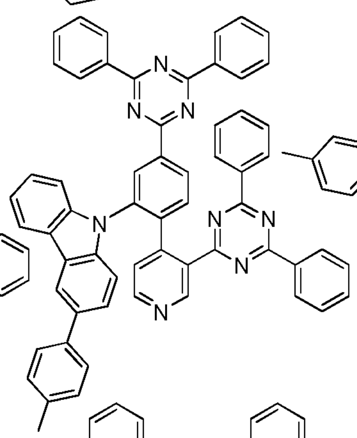
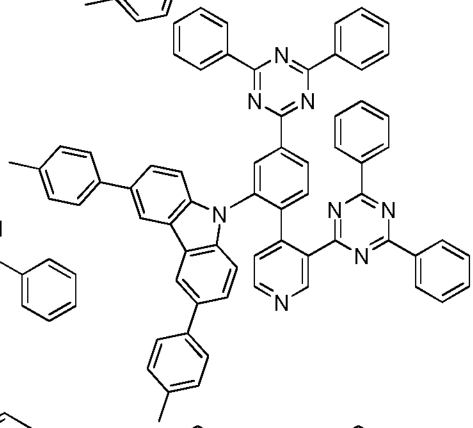
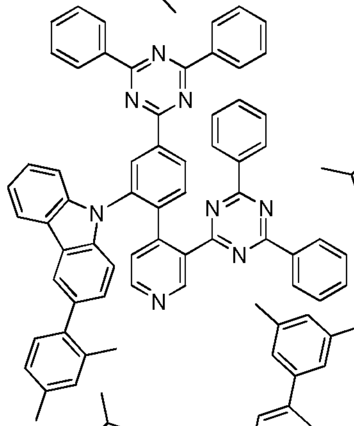
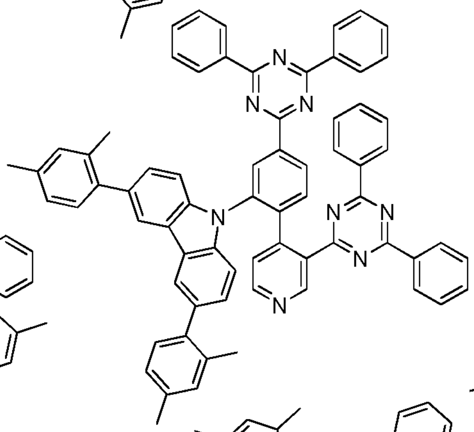
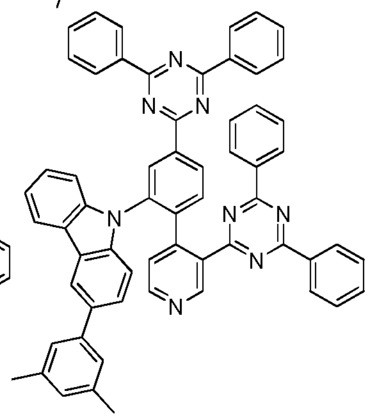
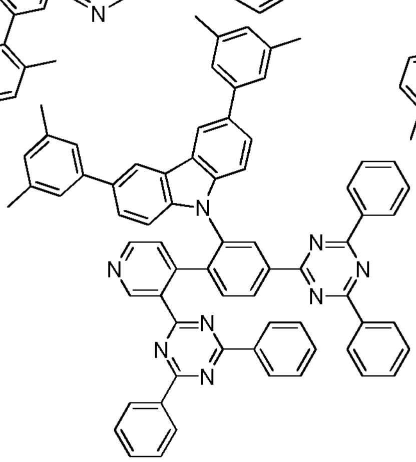
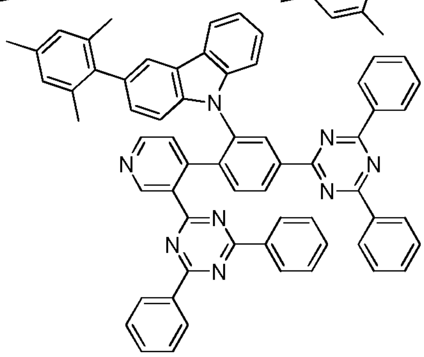
Example **2** was synthesized according to ***AAV1***, wherein 2-(4-fluoro-3-bromo-phenyl)-4,6-diphenyl-1,3,5-triazine was used as reactant (yield: 62%),
AAV2 wherein 3-bromo-5-chloropyridine (CAS 73583-39-8) was used as reactant (yield: 94%),
AAV3 (raw product used without further purification),
AAV4 (raw product used without further purification), wherein 2-chloro-4,6-diphenyl-1,3,5-triazine (CAS 3842-55-5) was used as reactant,
and ***AAV5*** , wherein 3,6-diphenyl-9H-carbazole (CAS 56525-79-2) was used as reactant (32 % yield).

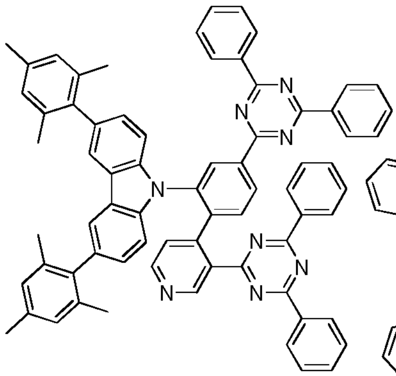
HPLC-MS: 26.88 min (934.43 m/z, 100 %).

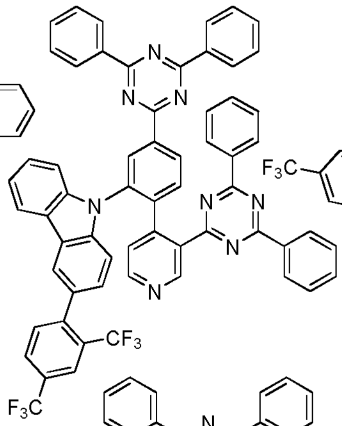
Figure 2 depicts the emission spectrum of example **2** (10 % by weight in PMMA). The emission maximum (λ_{max}) is at 463 nm. The photoluminescence quantum yield (PLQY) is 51 %, the full width at half maximum (FWHM) is 0.42 eV. The resulting CIE_x coordinate is determined at 0.16 and the CIE_y coordinate at 0.19. The emission lifetime is 9 µs and the energy of the highest occupied molecular orbital (E^{HOMO}) is -6.0 eV.

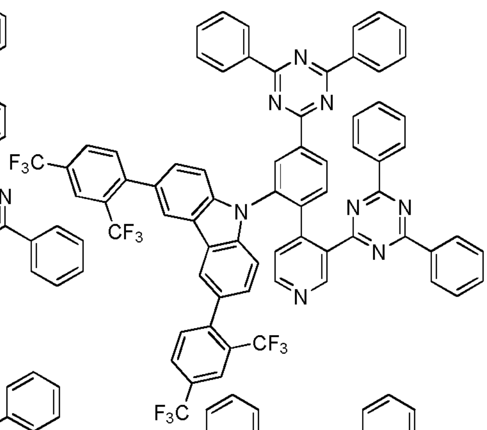
Additional examples of organic molecules of the invention

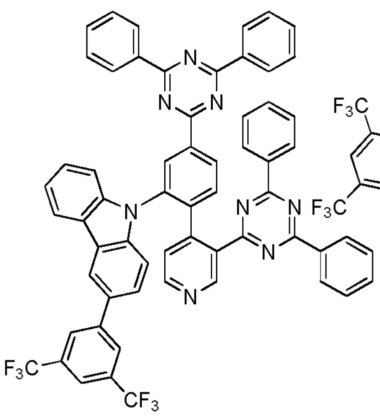













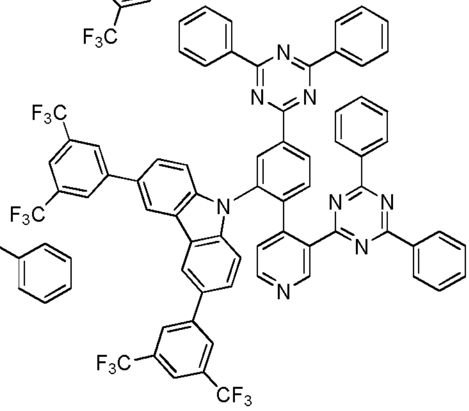












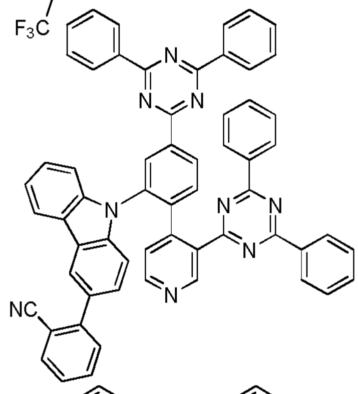


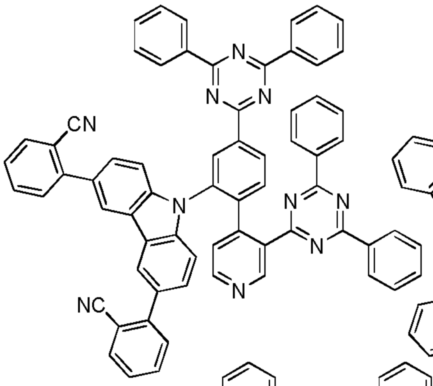


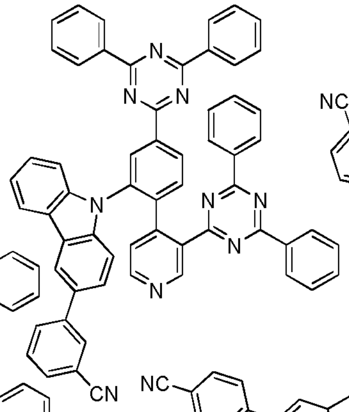


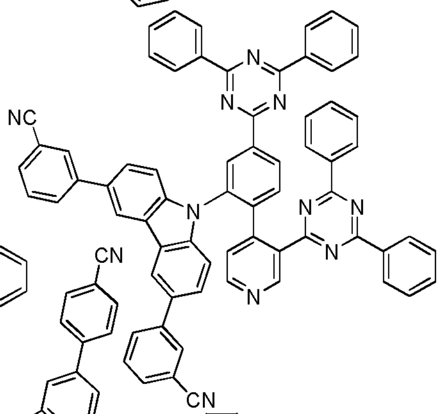


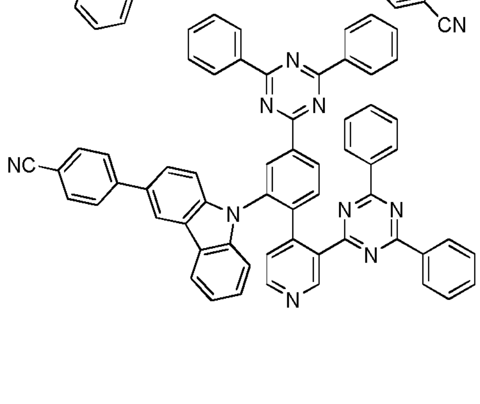


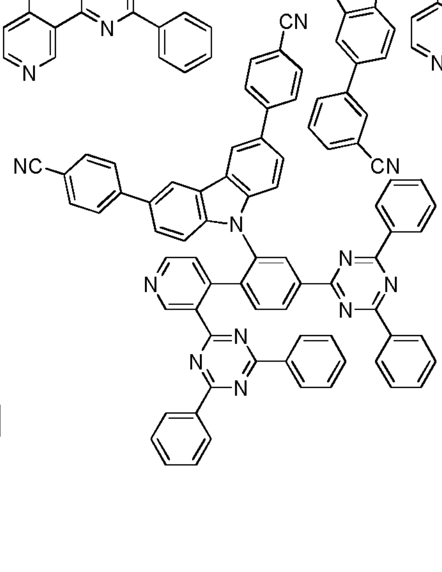


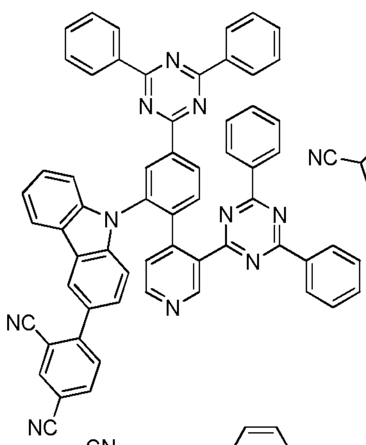
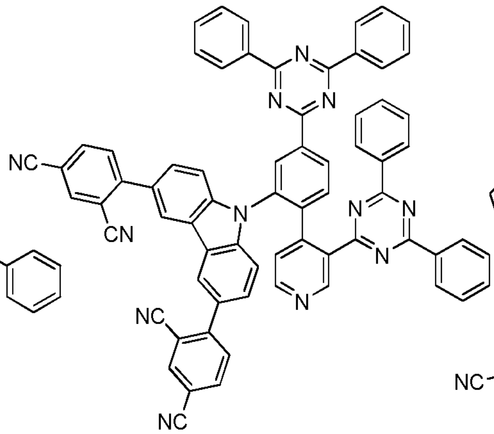
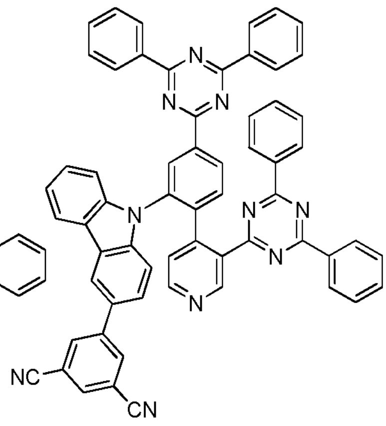
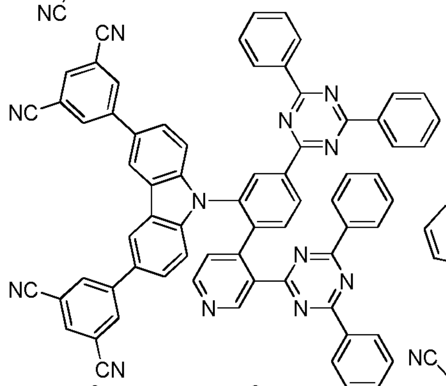
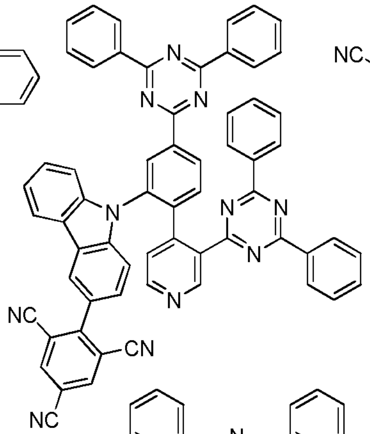
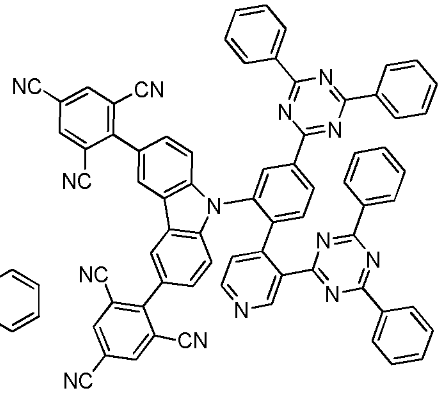
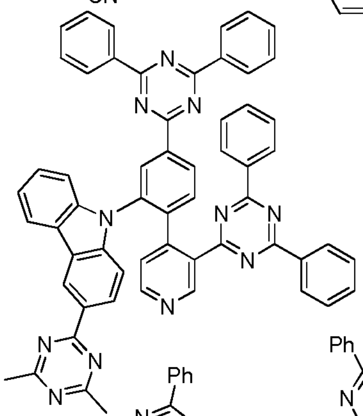
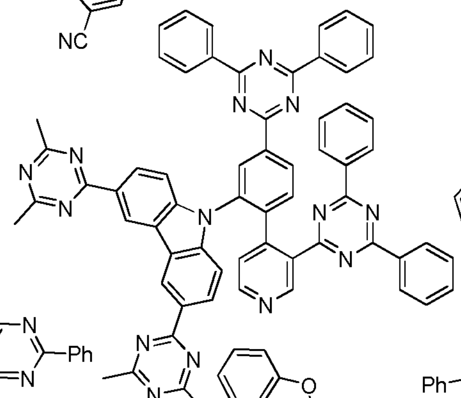
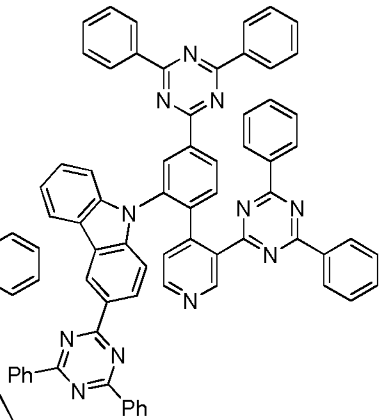
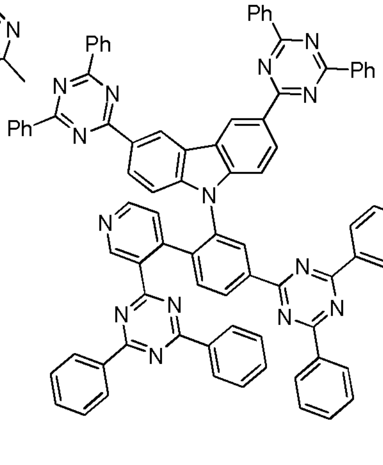
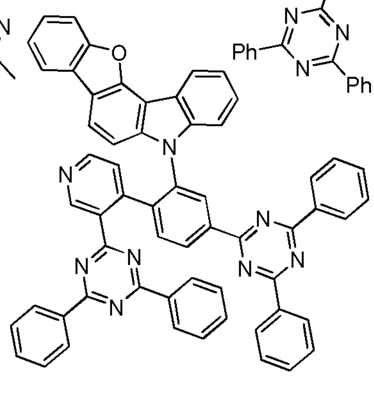


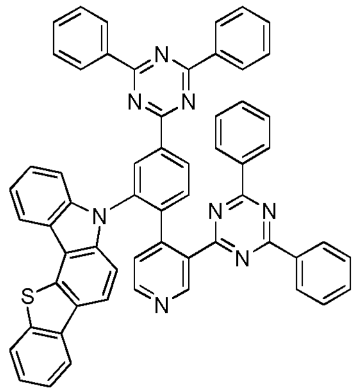
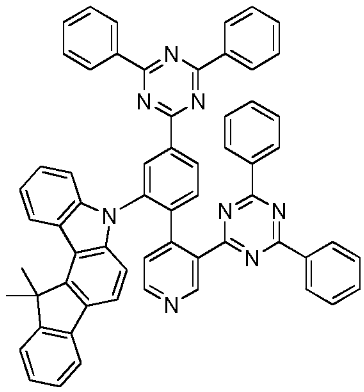
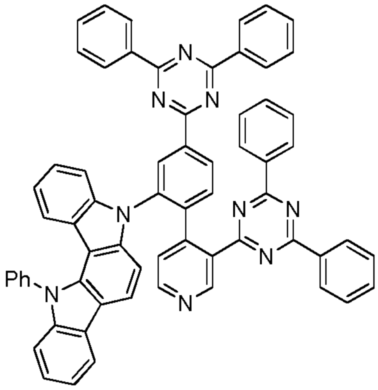
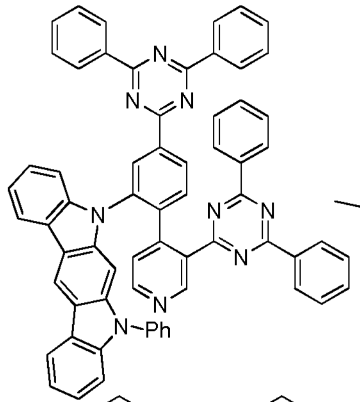
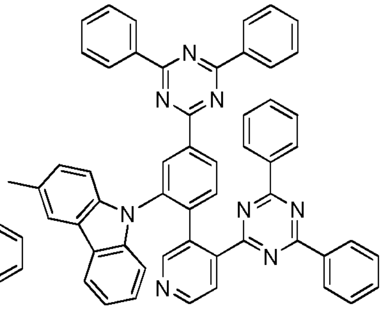
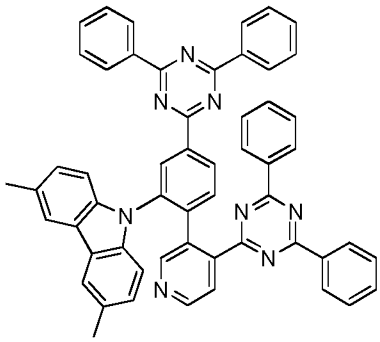
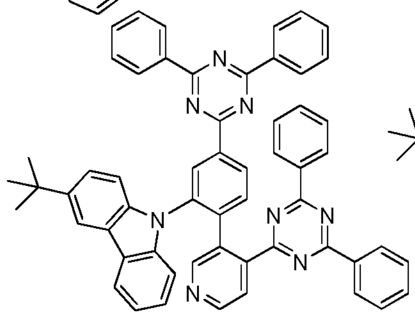
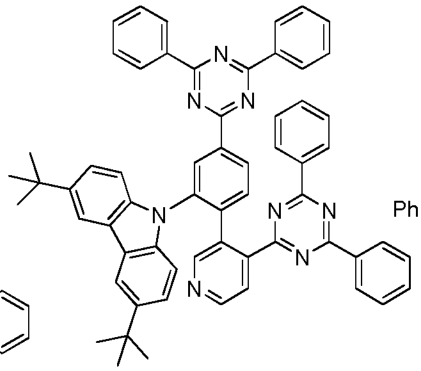
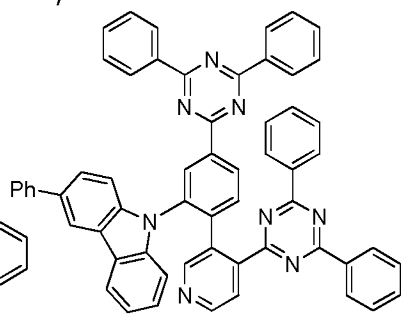
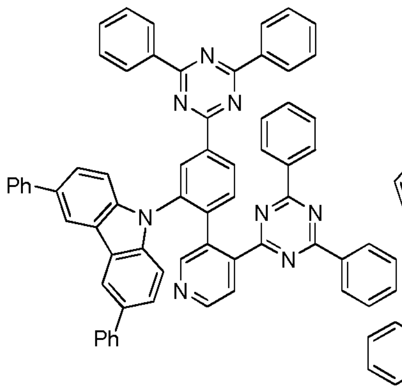
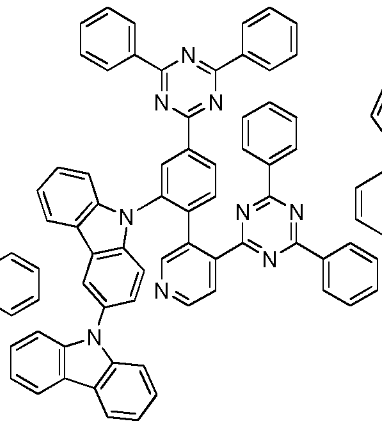
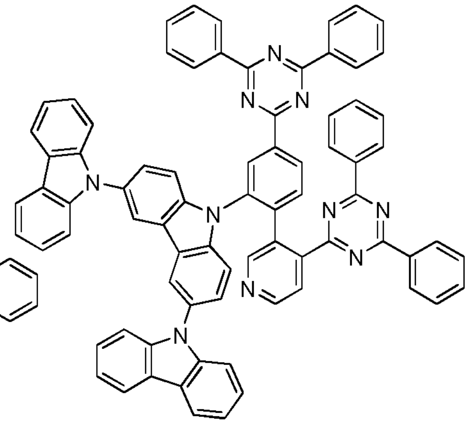


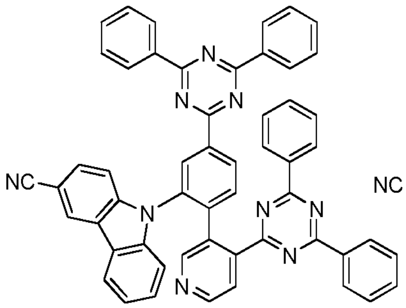
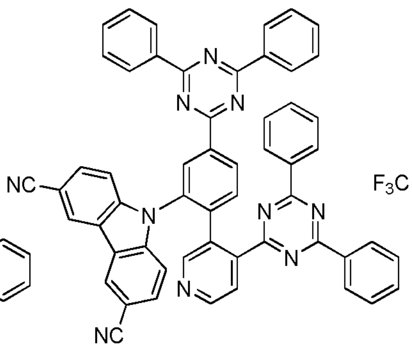
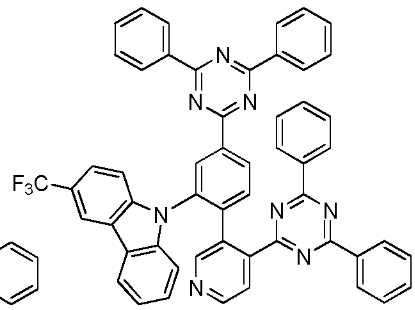
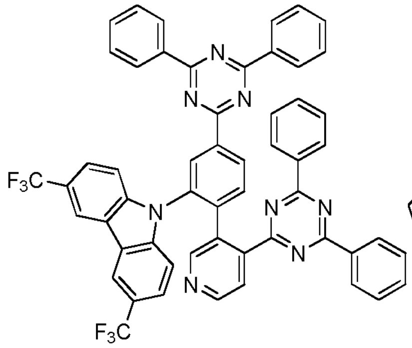
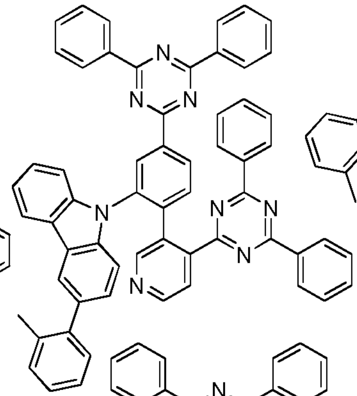
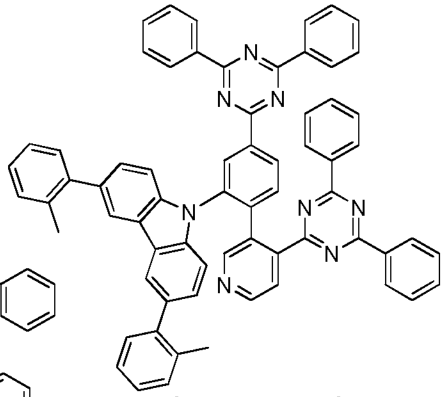
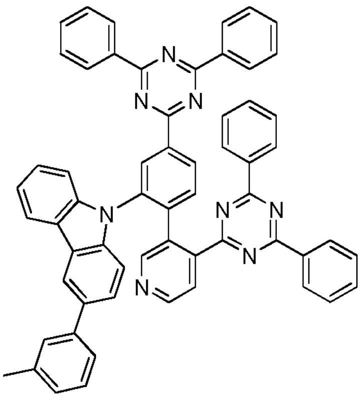
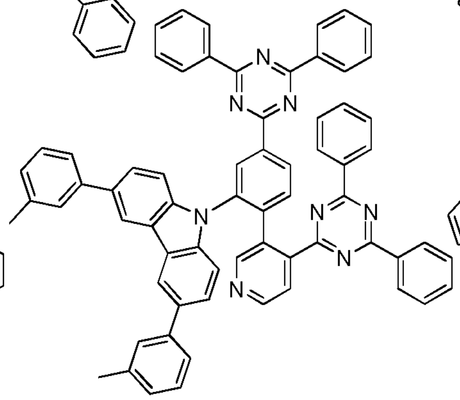
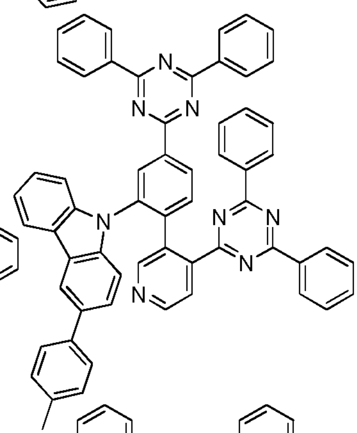
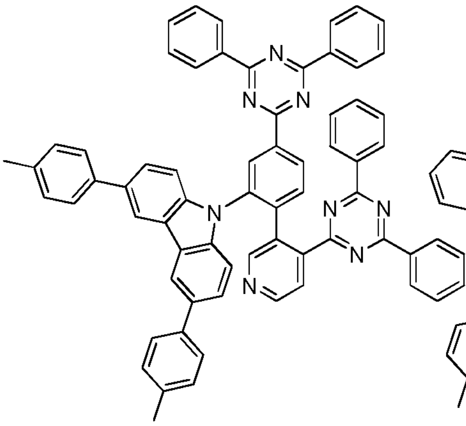
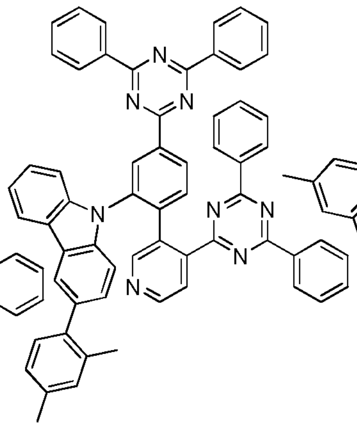
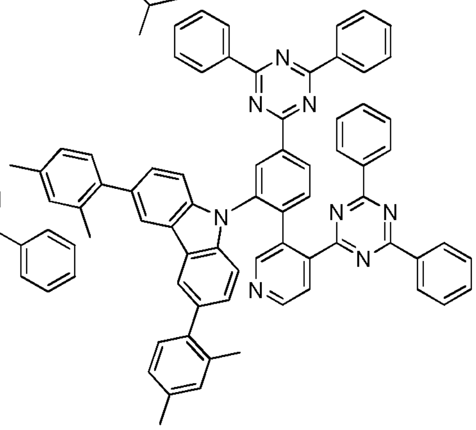


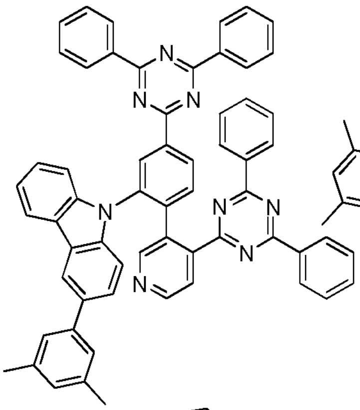
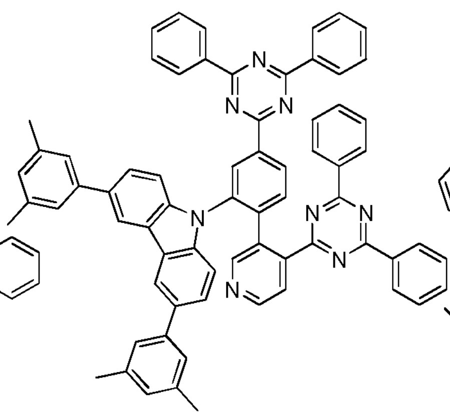
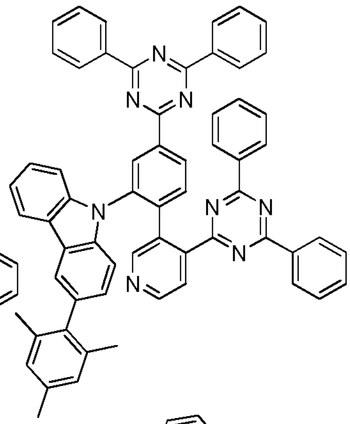
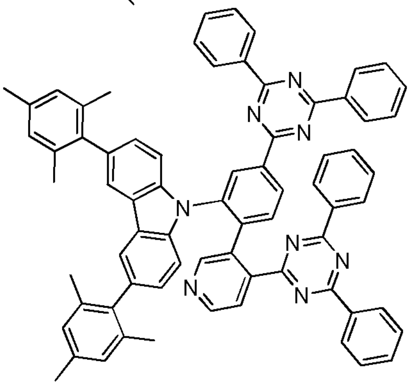
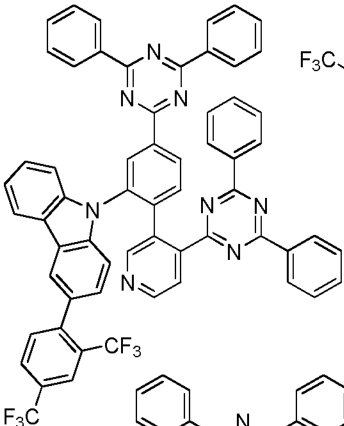
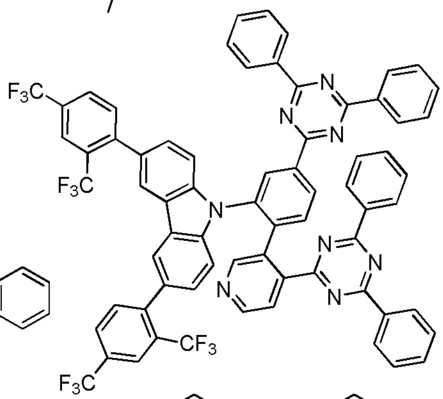
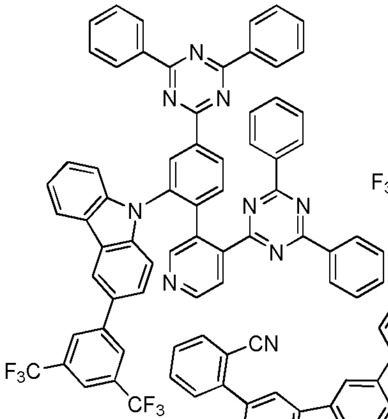
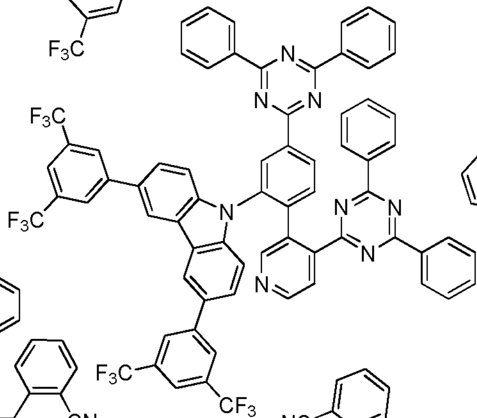
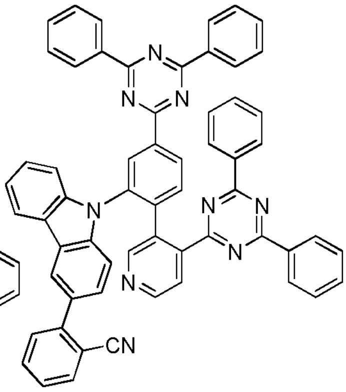
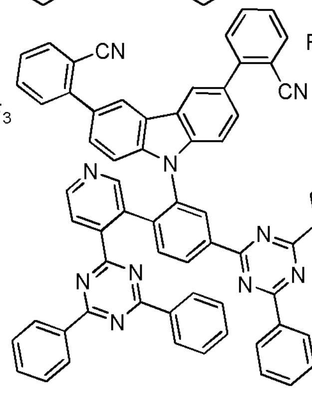
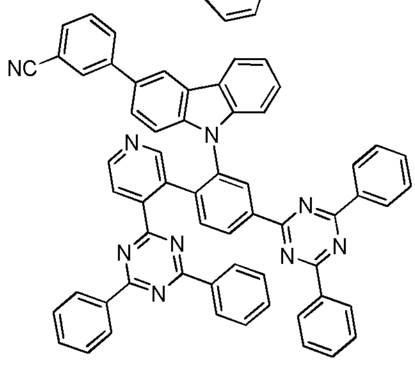


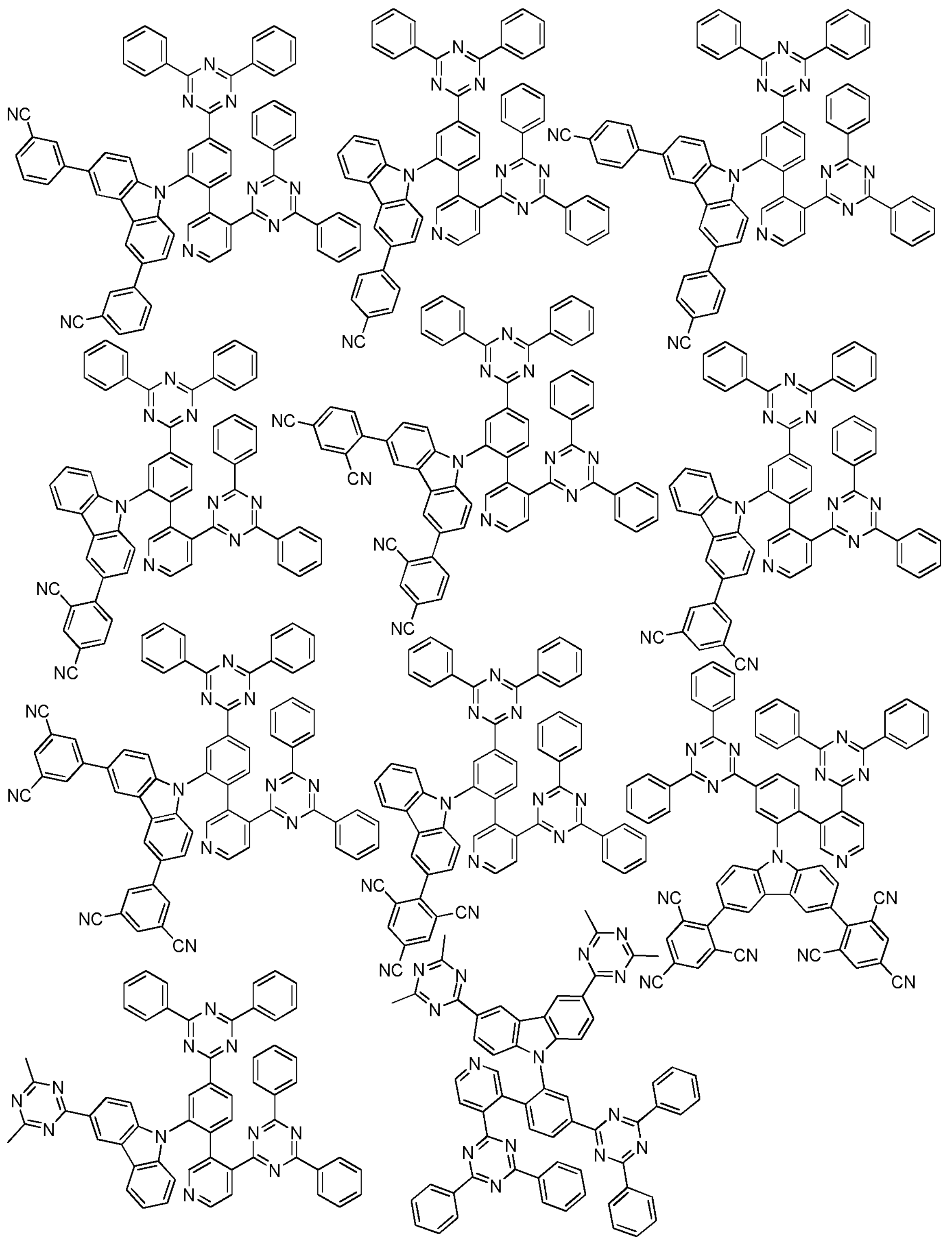


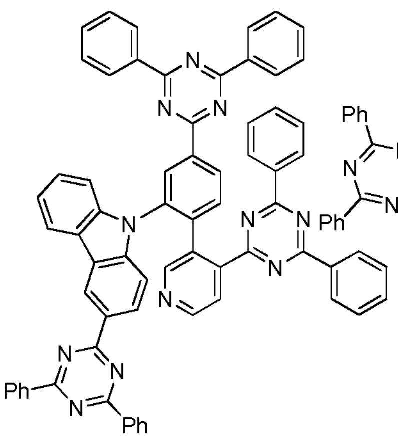
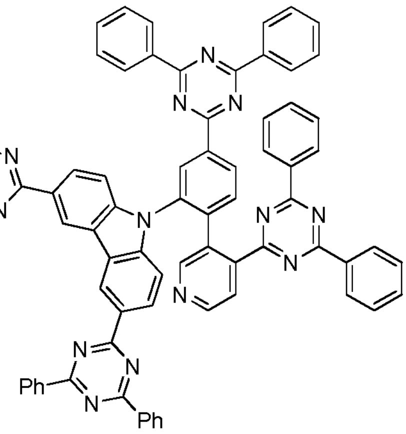
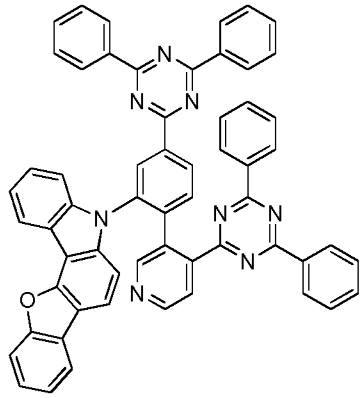
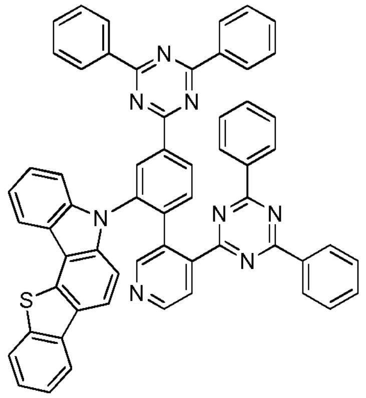
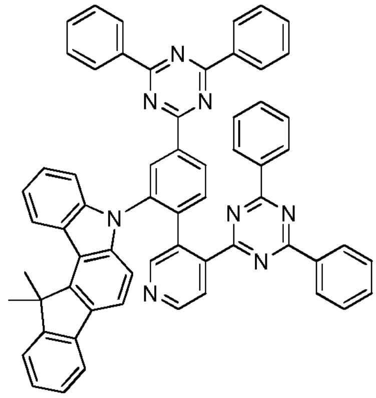
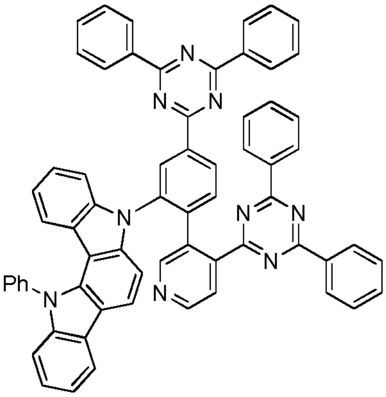
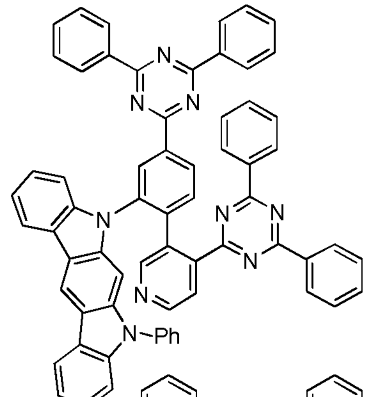
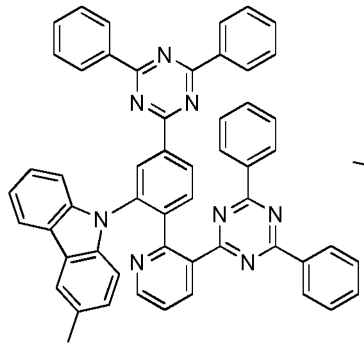
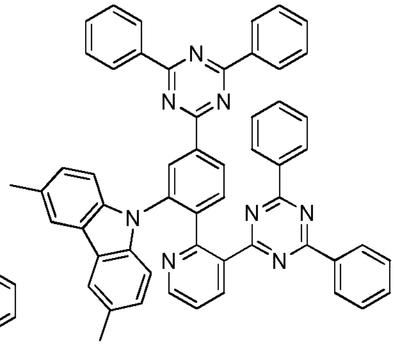
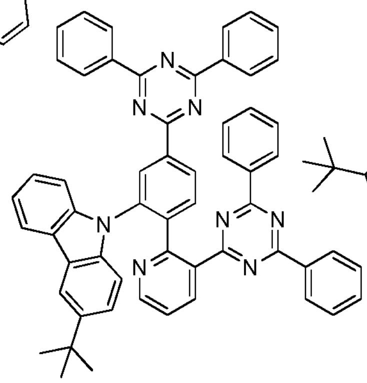
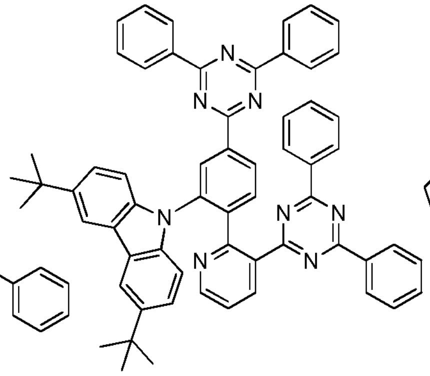
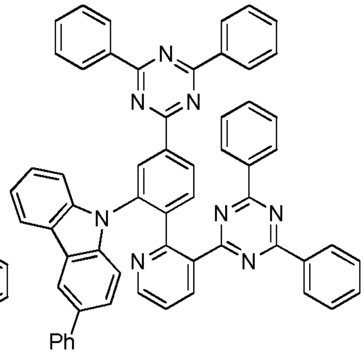












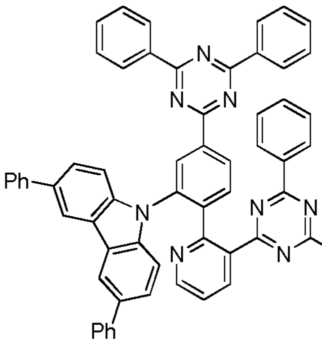













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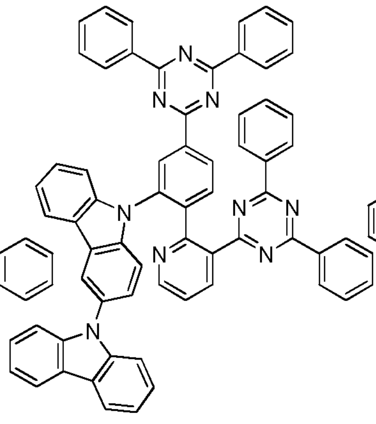
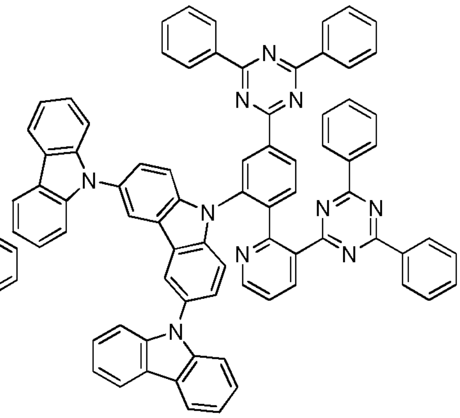
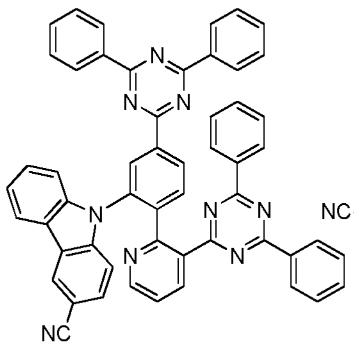
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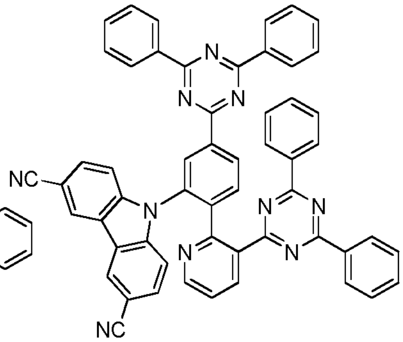
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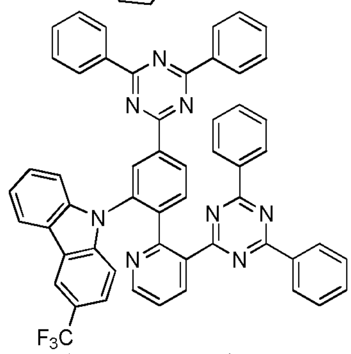
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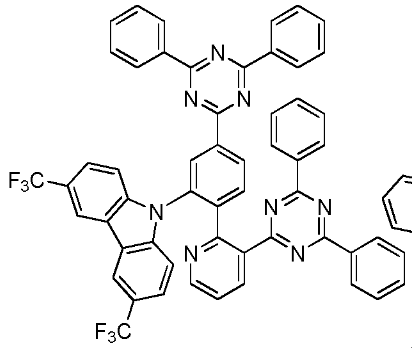
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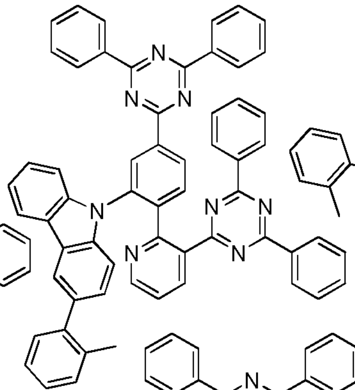
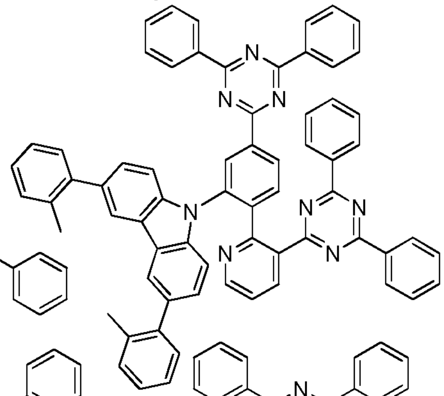
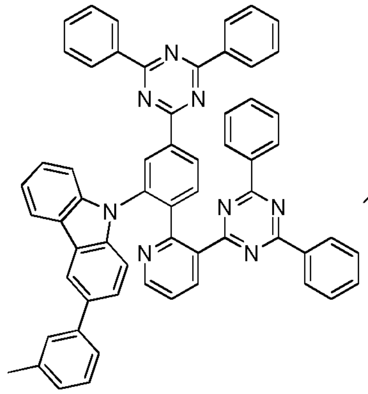
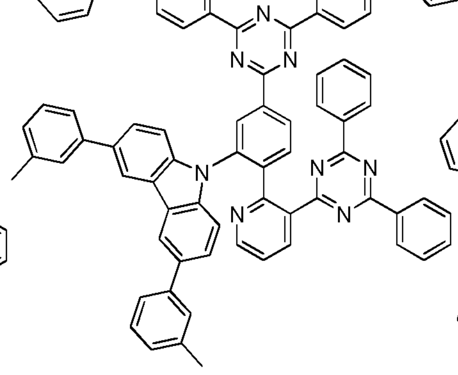
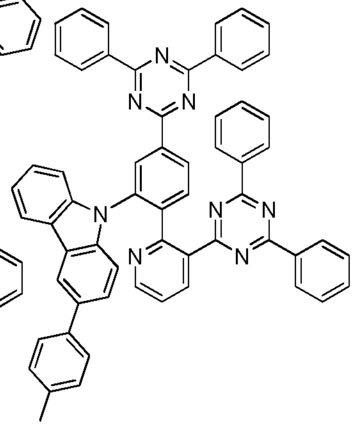

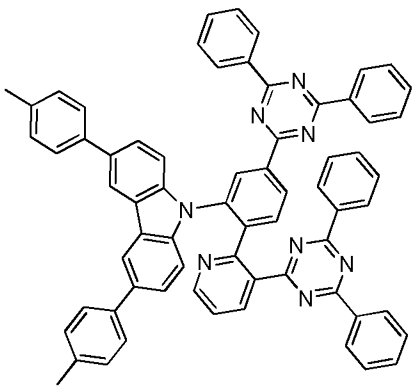
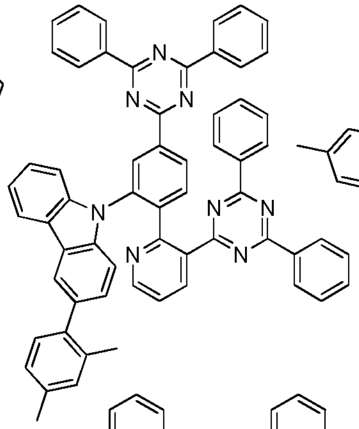
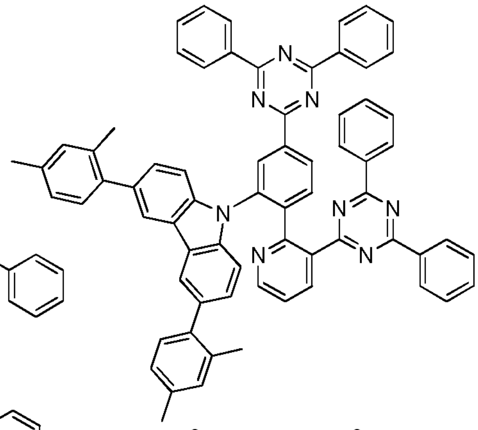
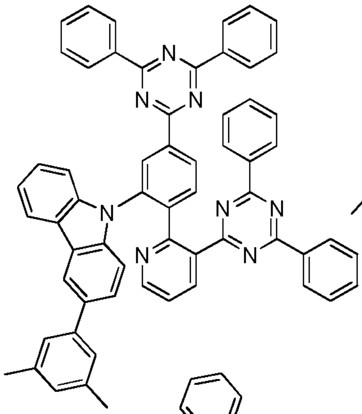
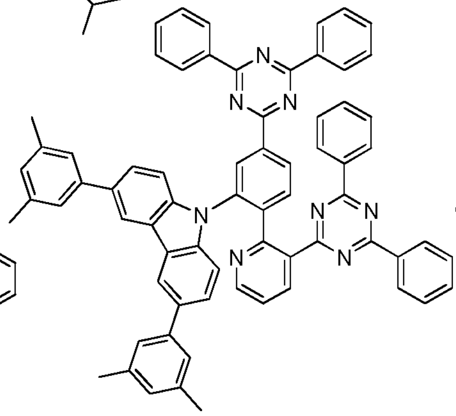
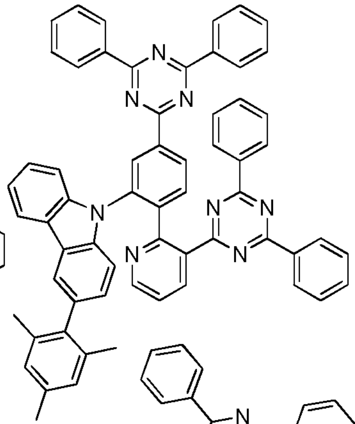
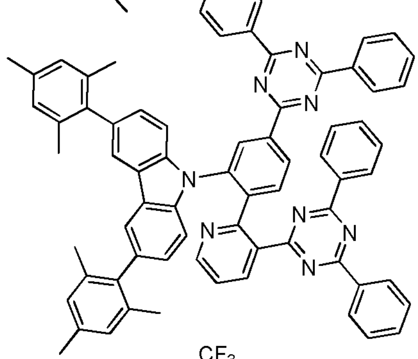
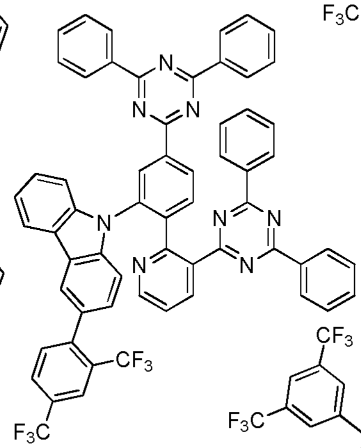
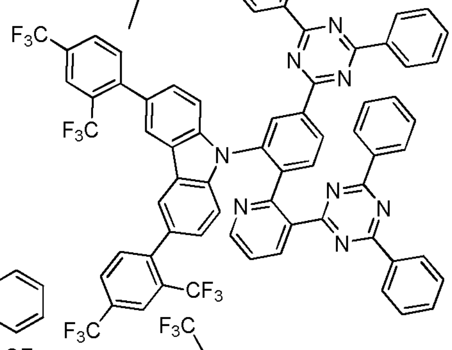
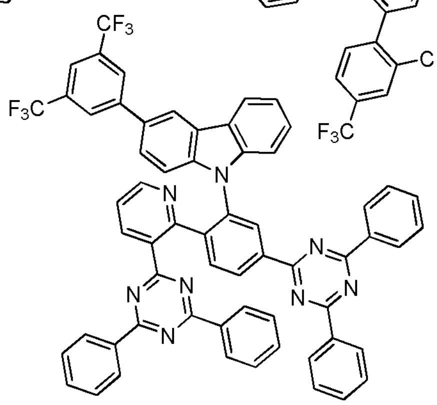
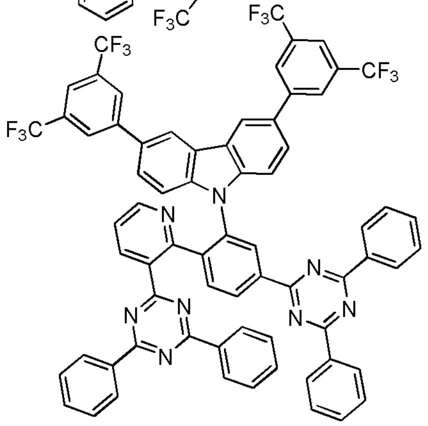

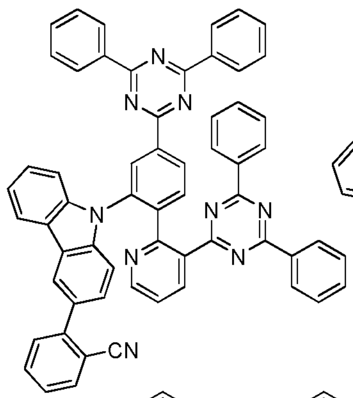
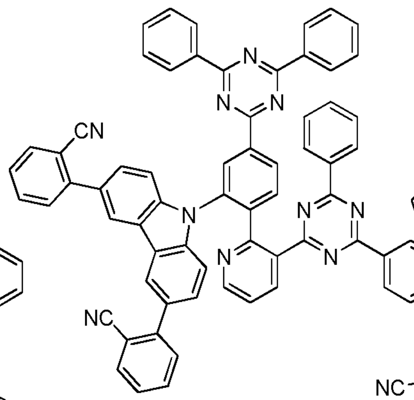
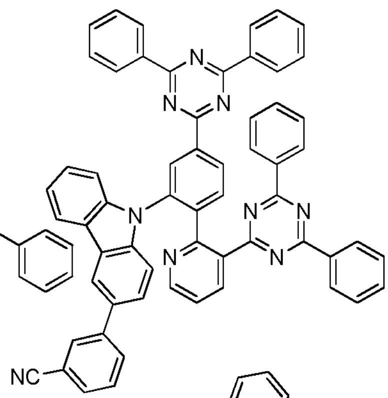
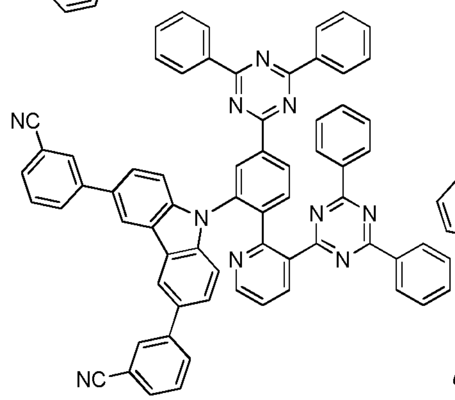
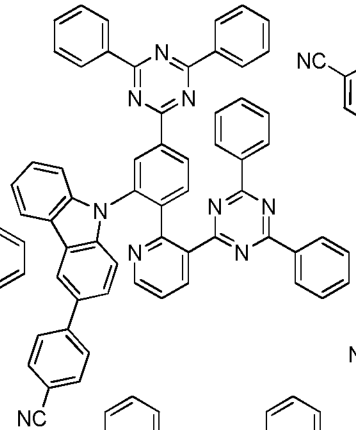
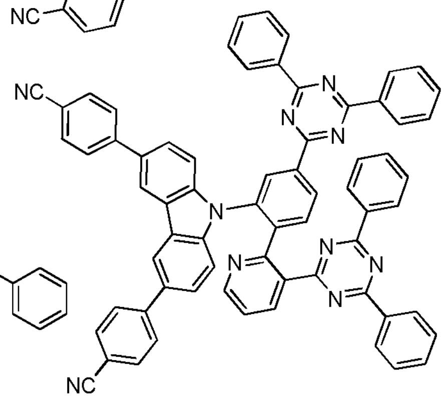
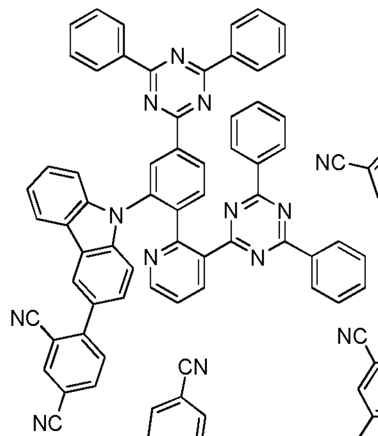
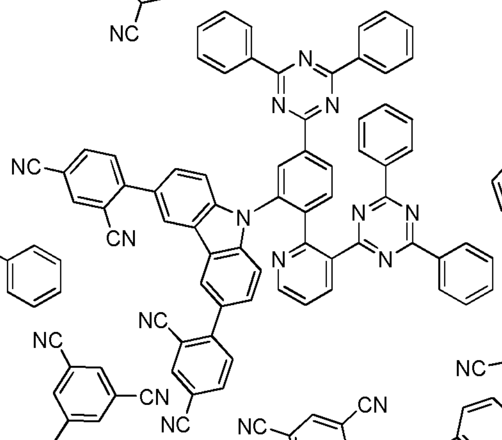
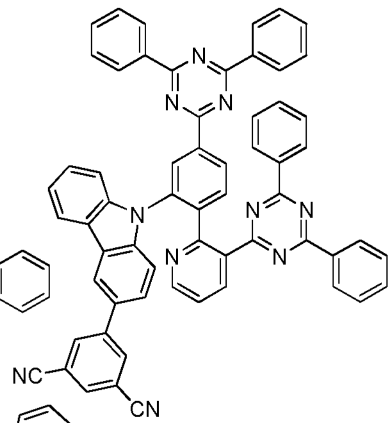
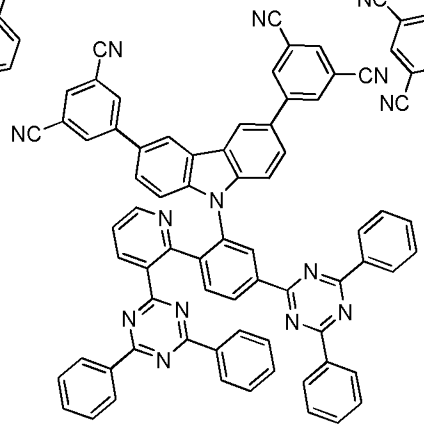
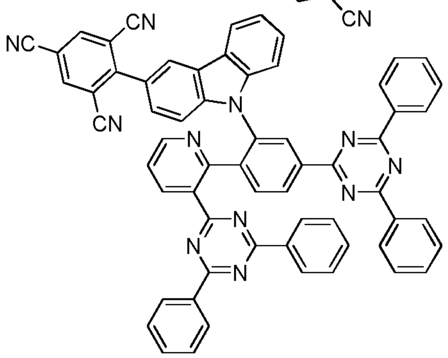

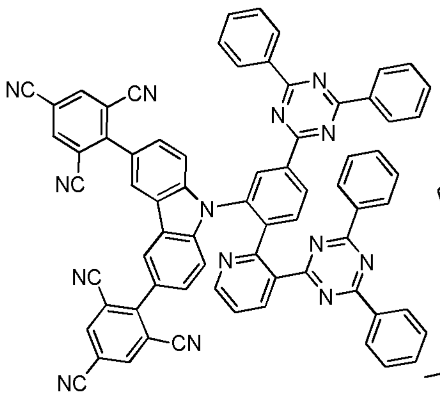

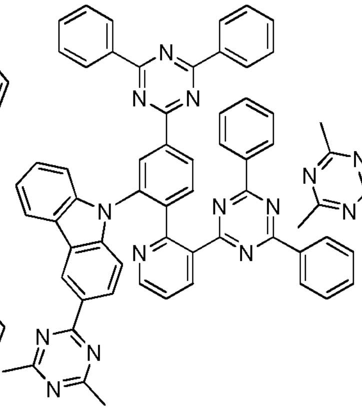

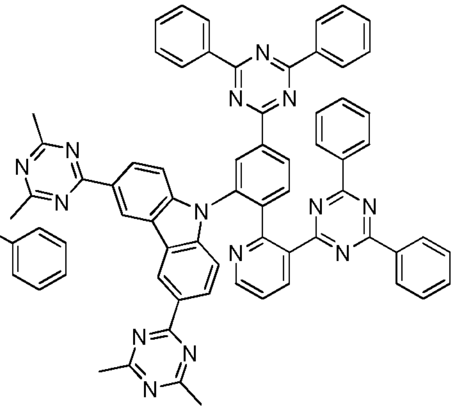

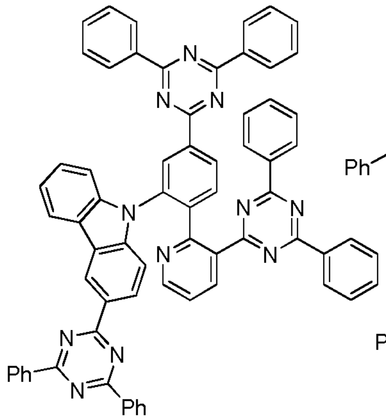

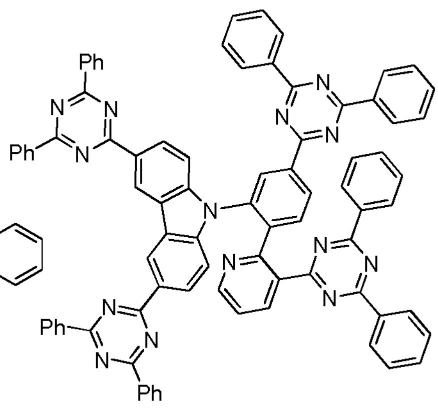

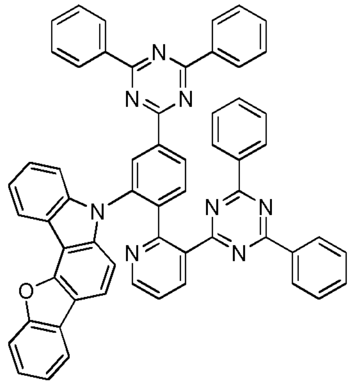

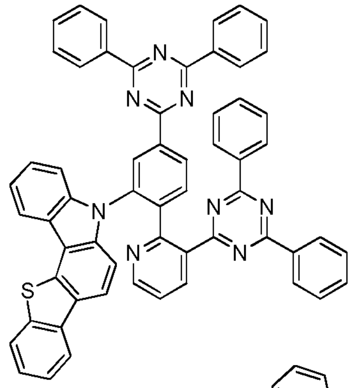

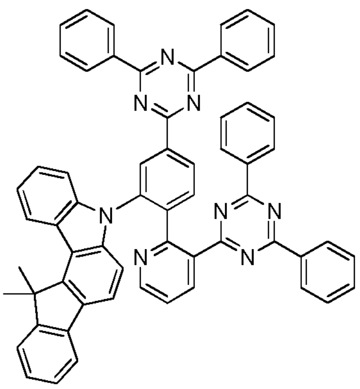

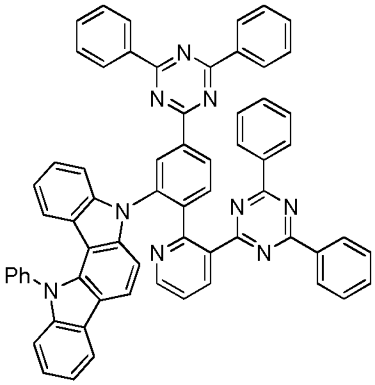

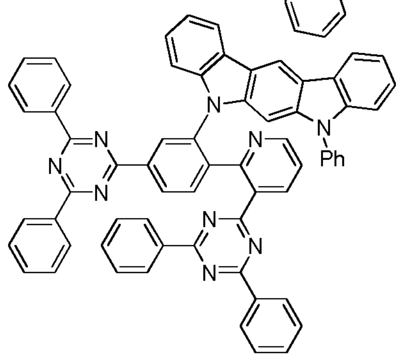

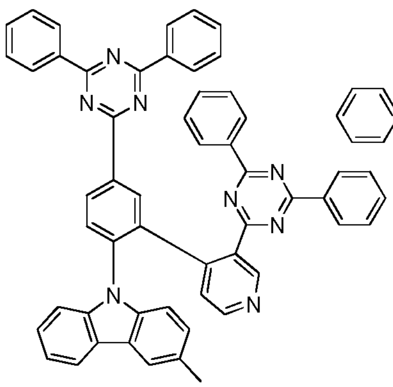
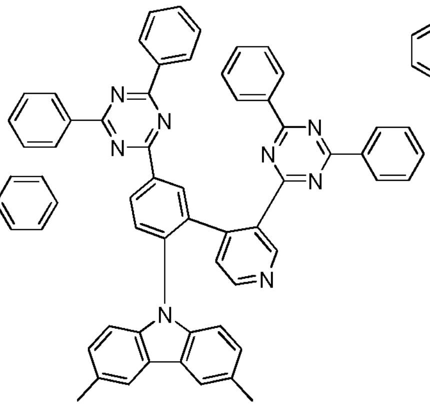
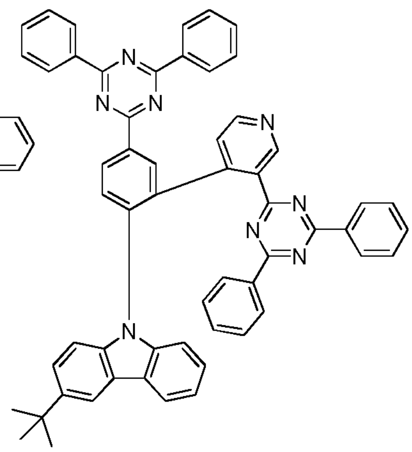
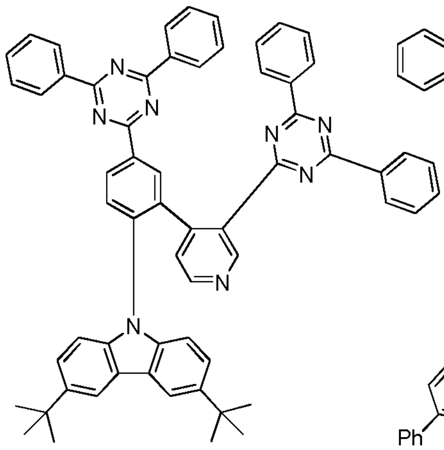
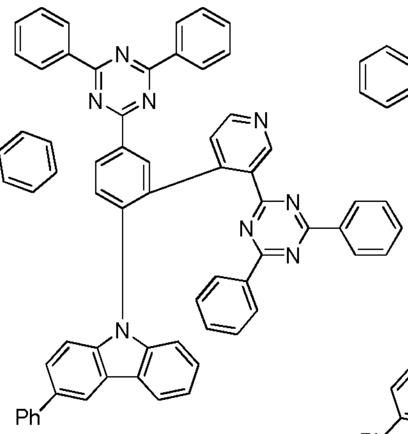
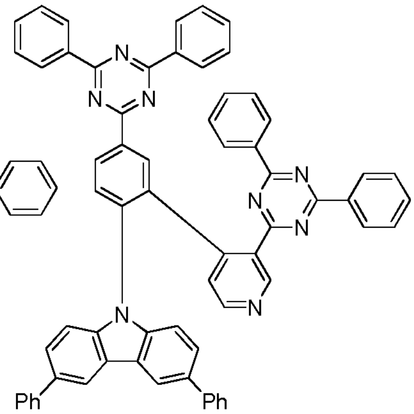
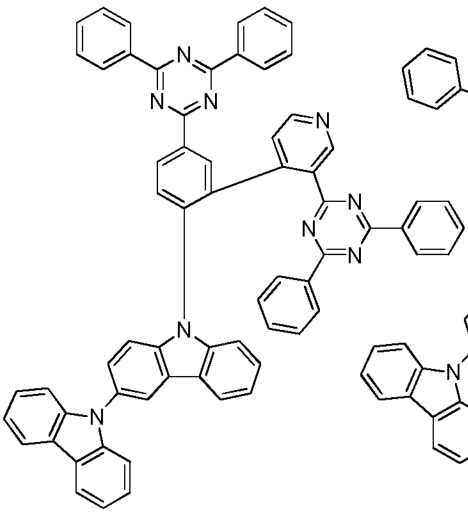
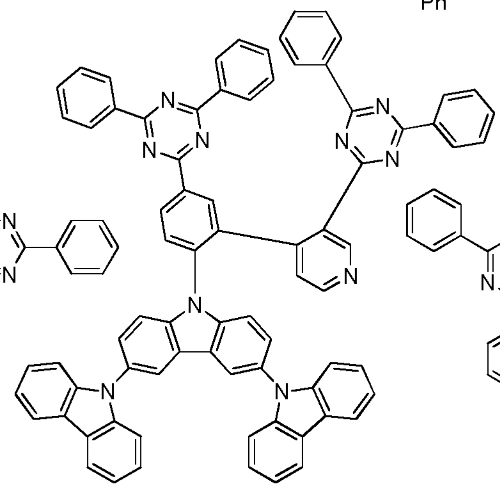
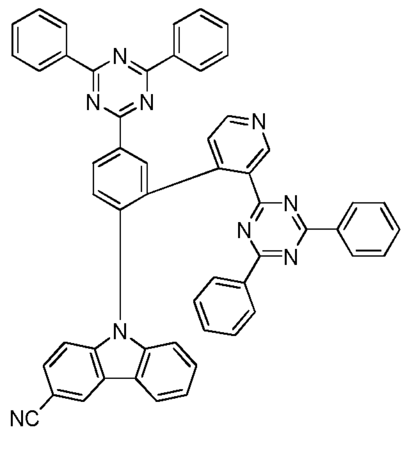

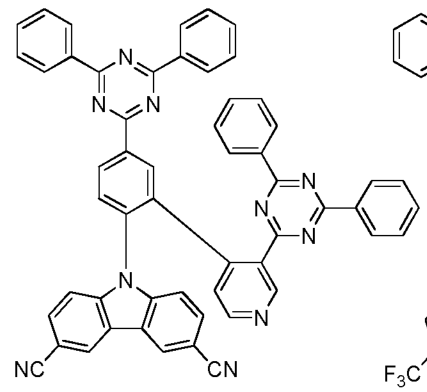

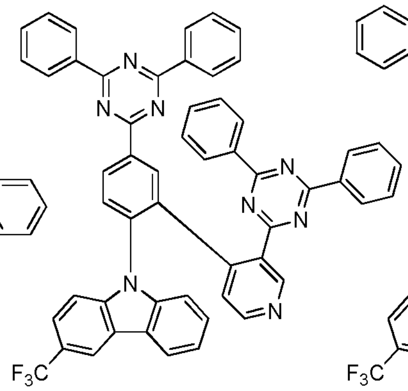

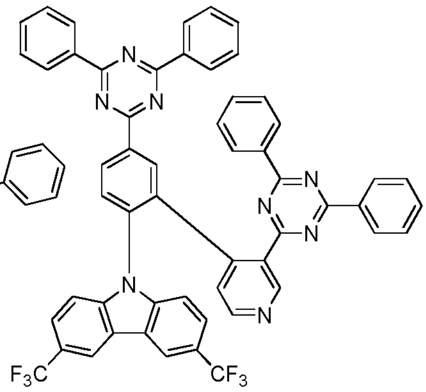

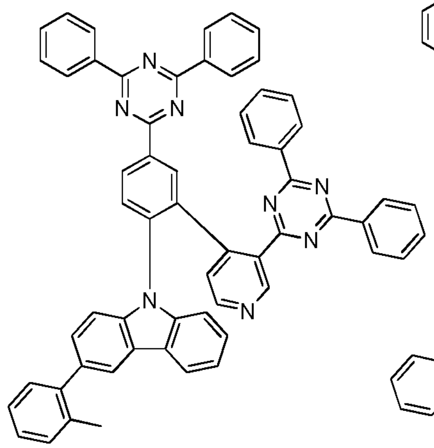

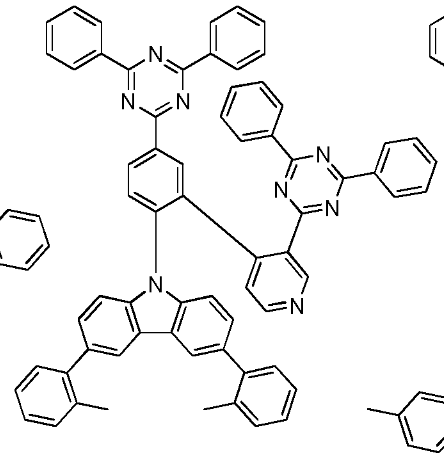

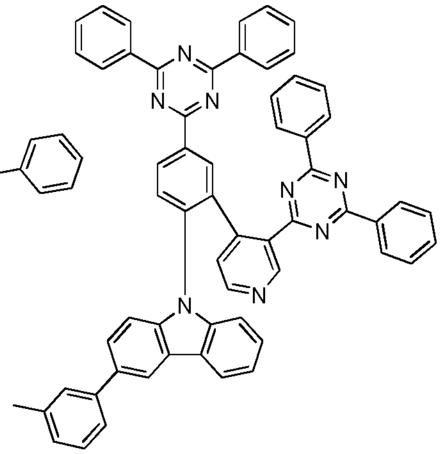

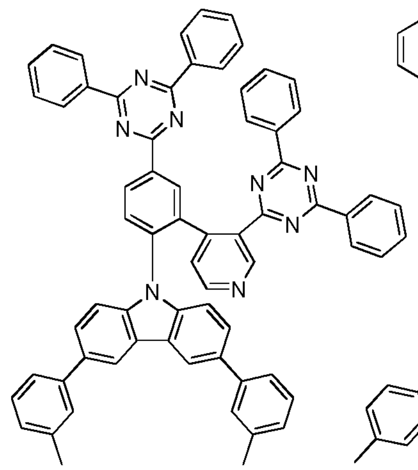

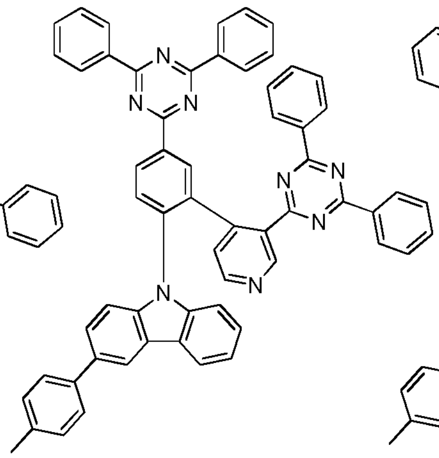

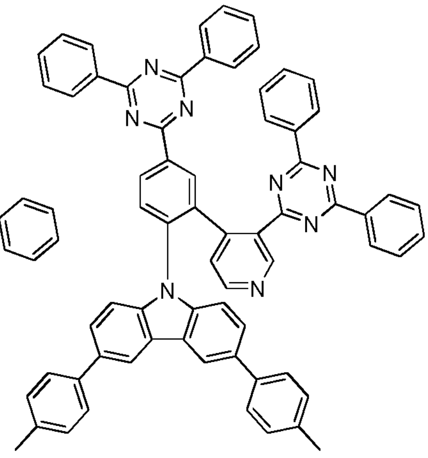

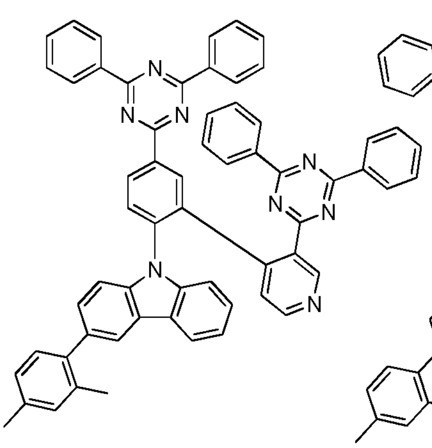
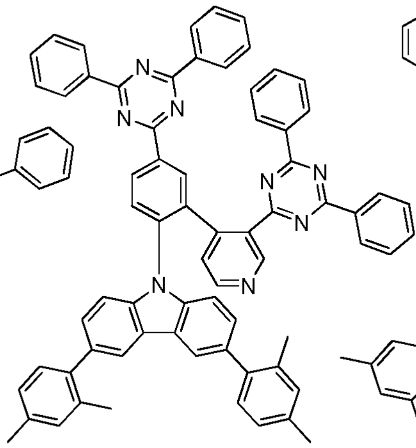
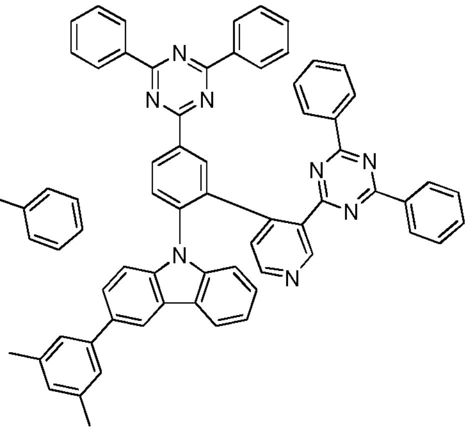

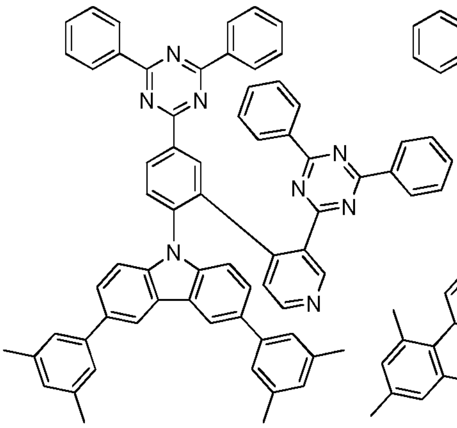
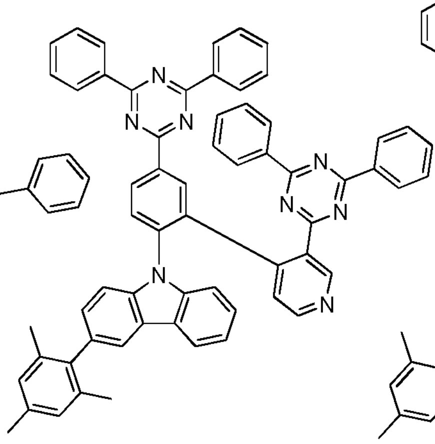
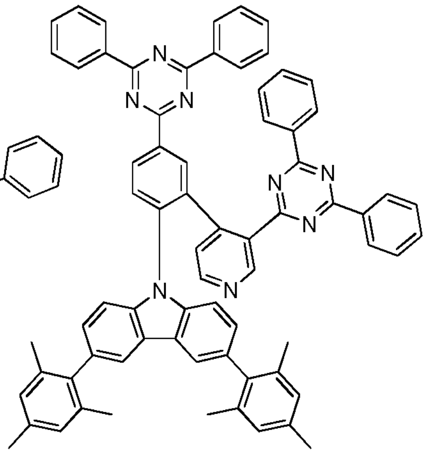

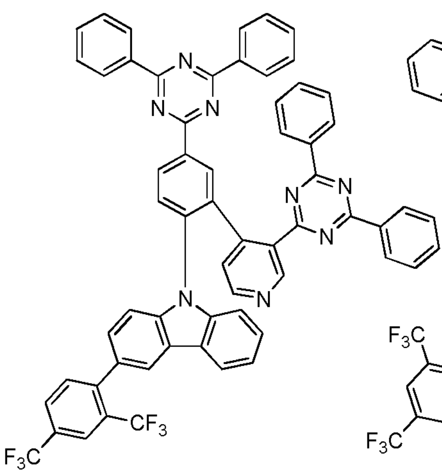
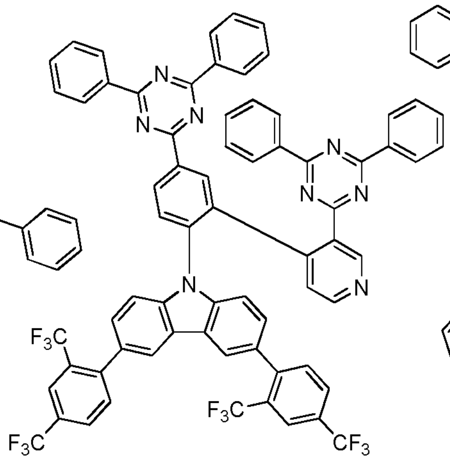
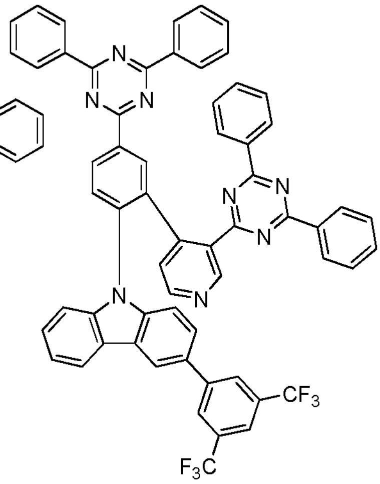

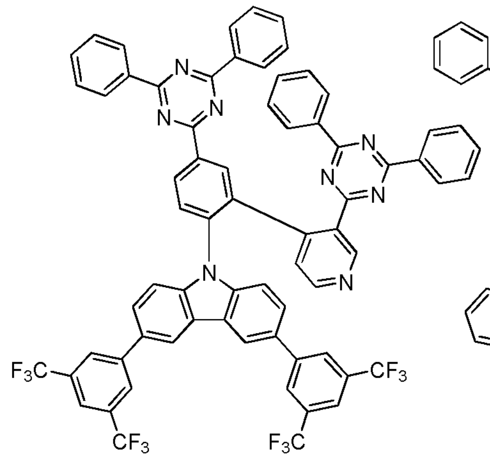

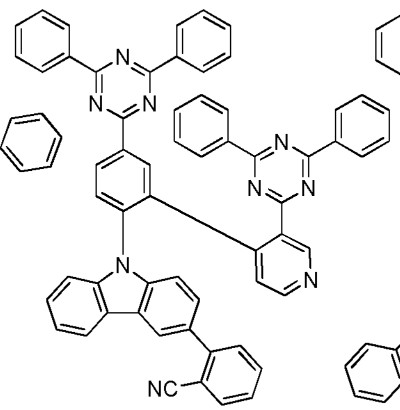

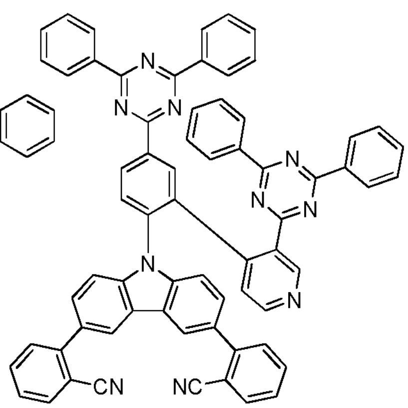

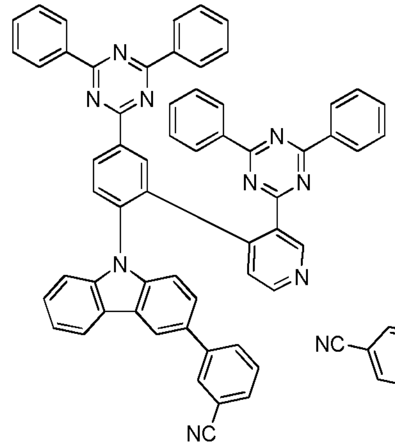

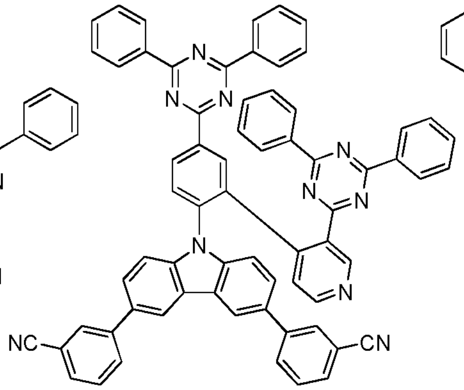

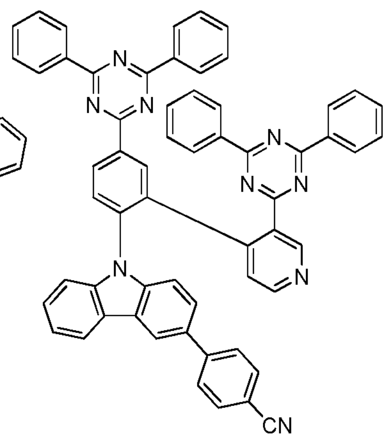

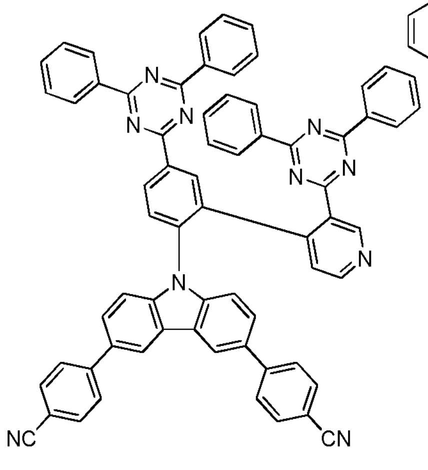

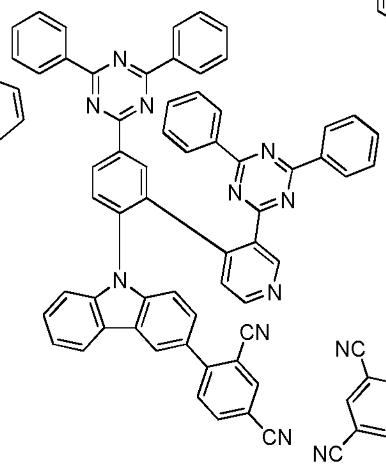

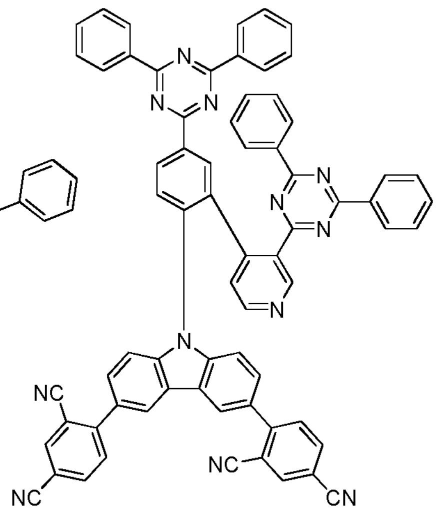

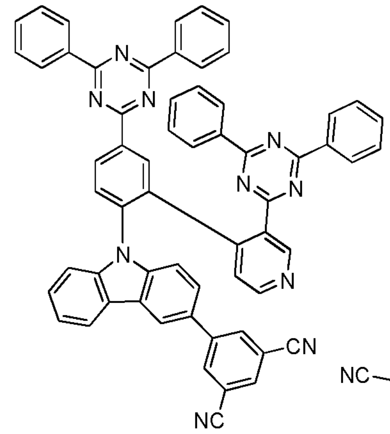

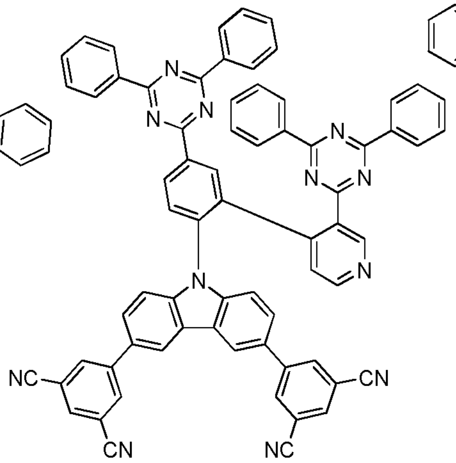

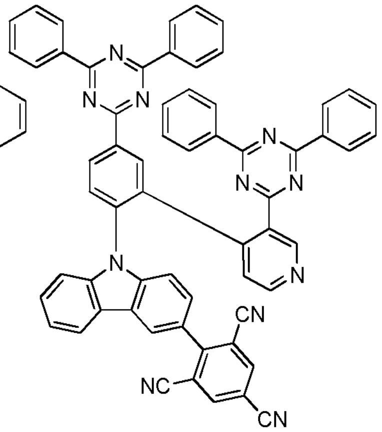

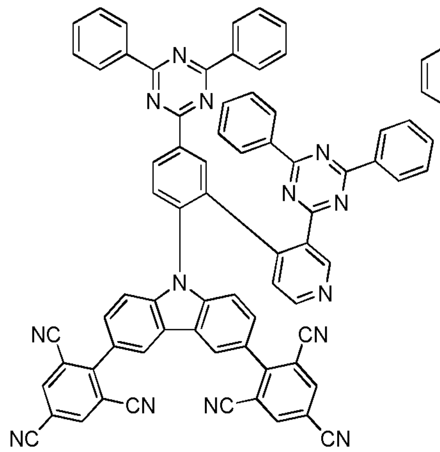

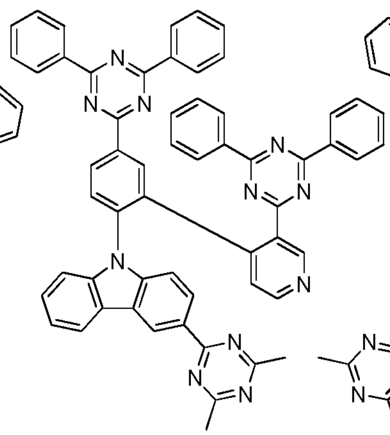

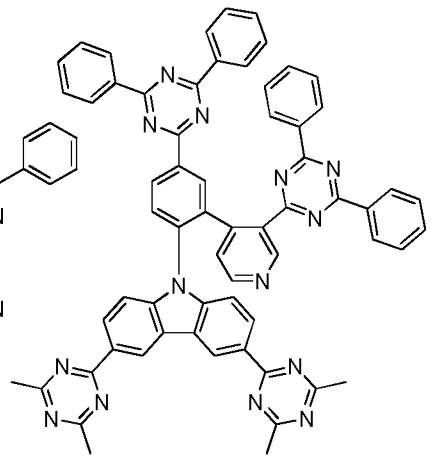

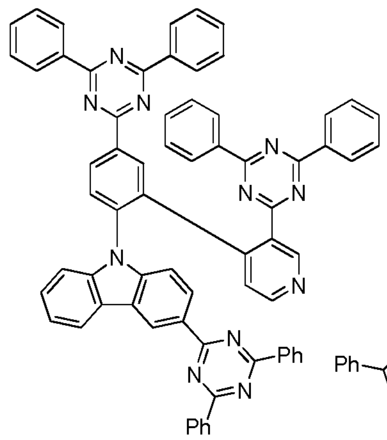

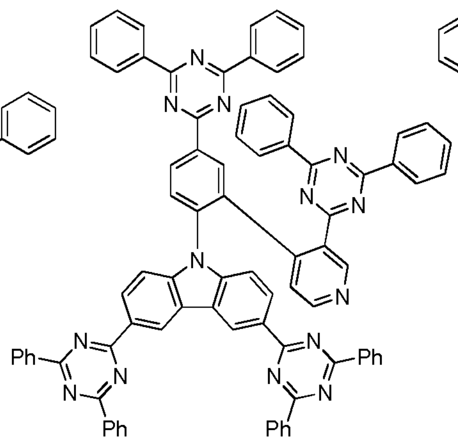

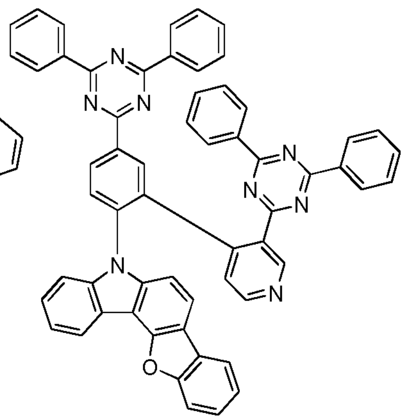

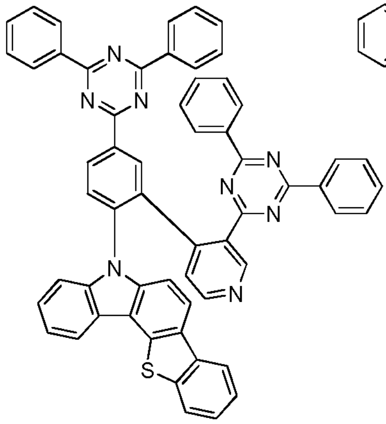
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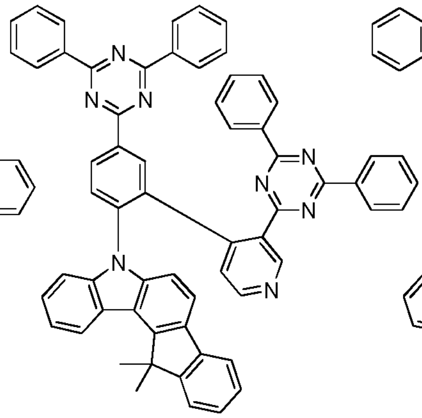

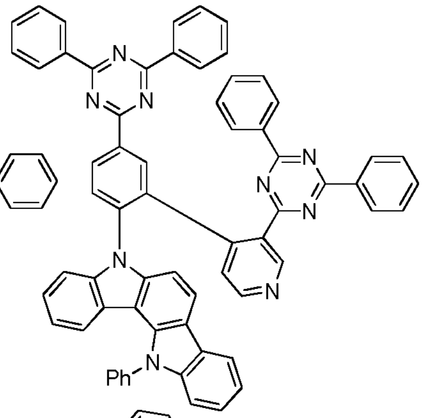
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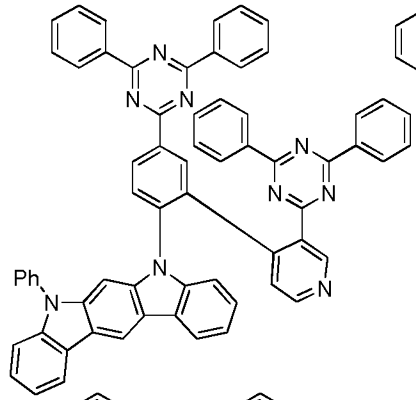
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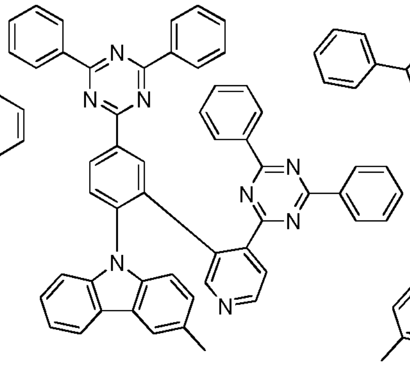

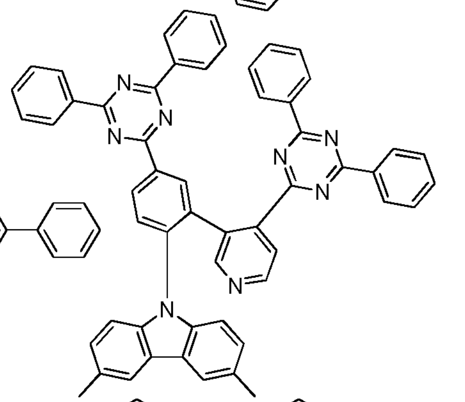

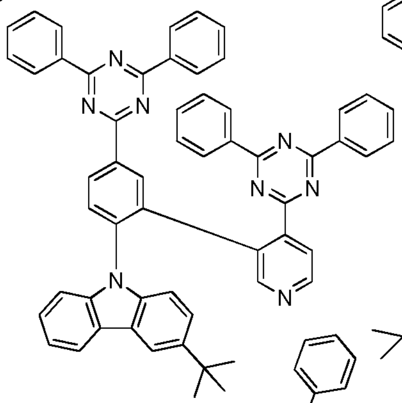

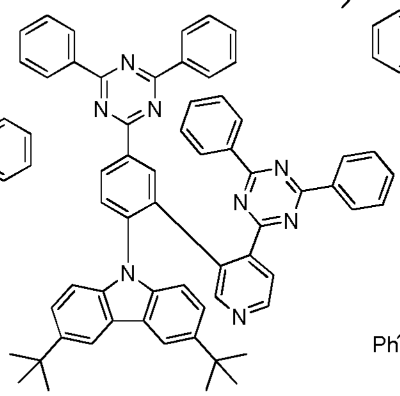

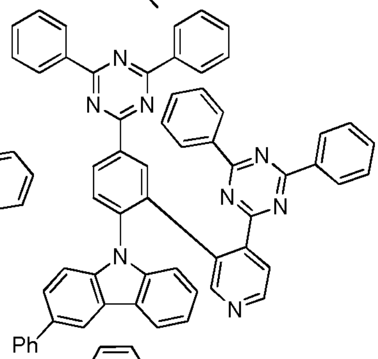
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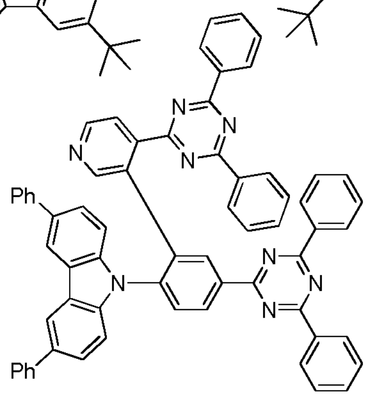
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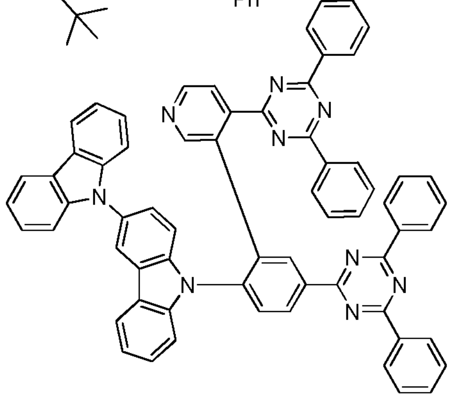

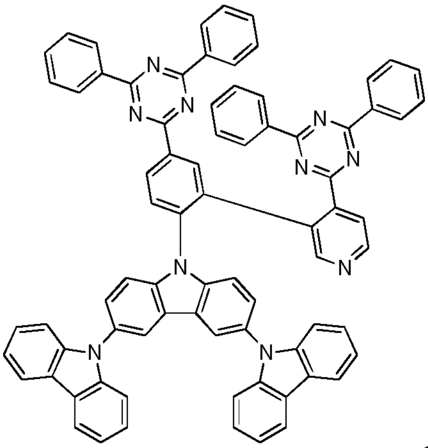

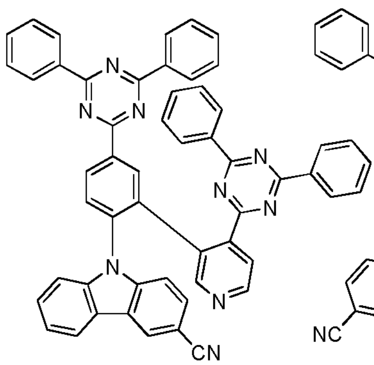

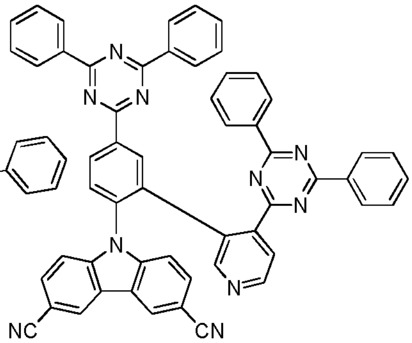

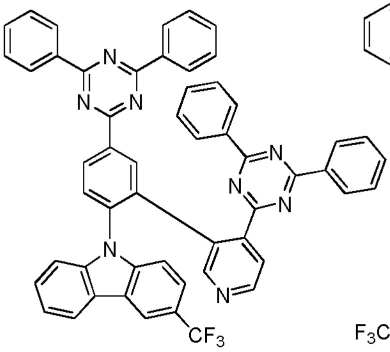

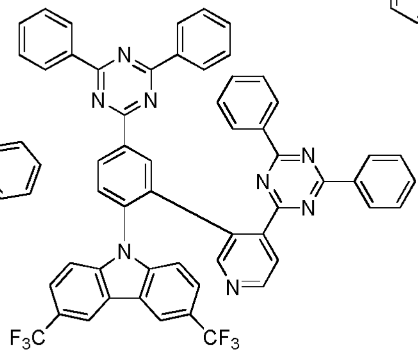

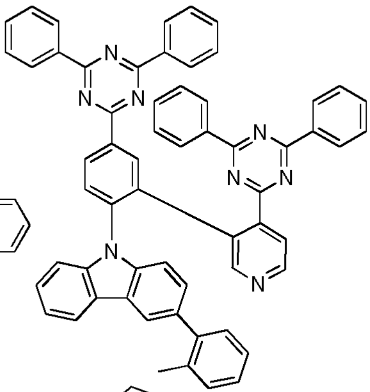

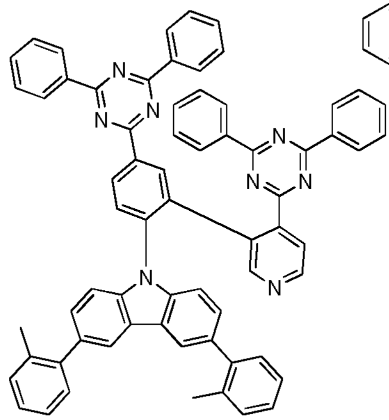

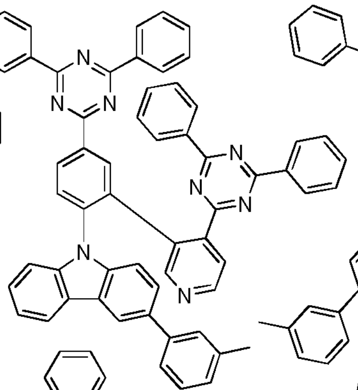

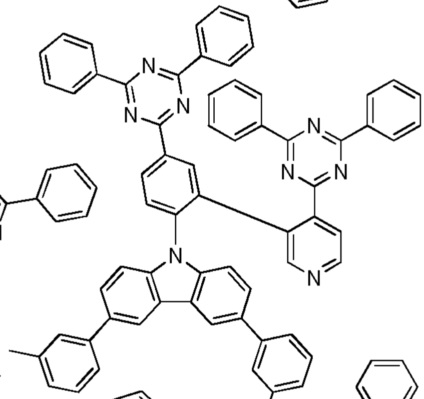

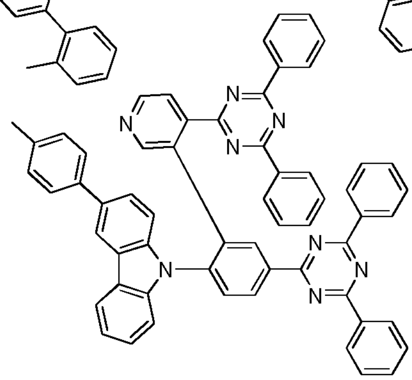

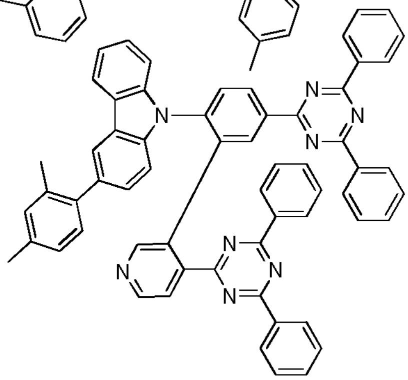

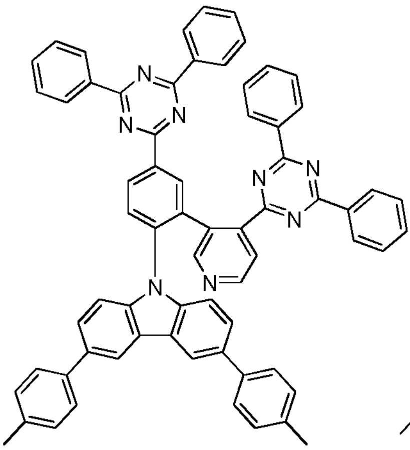

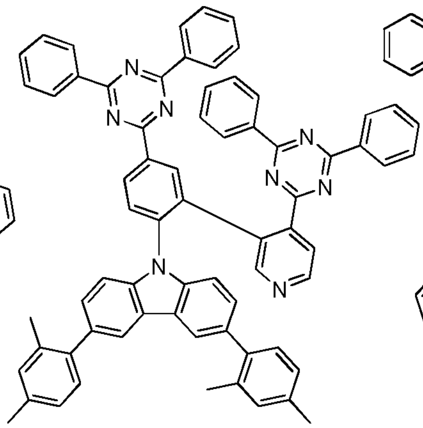

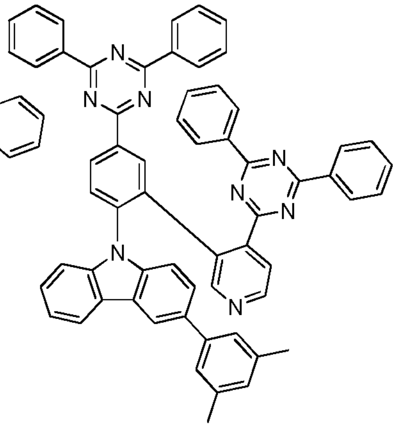

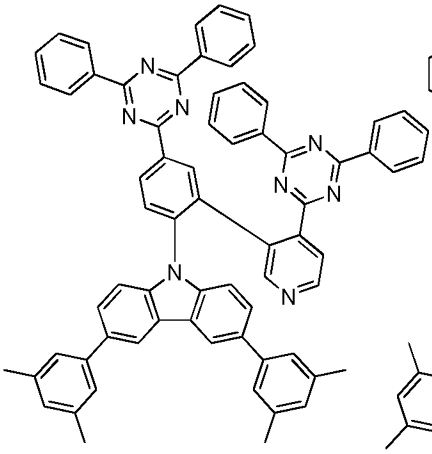

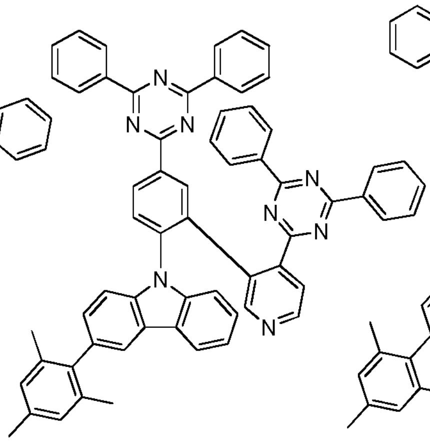

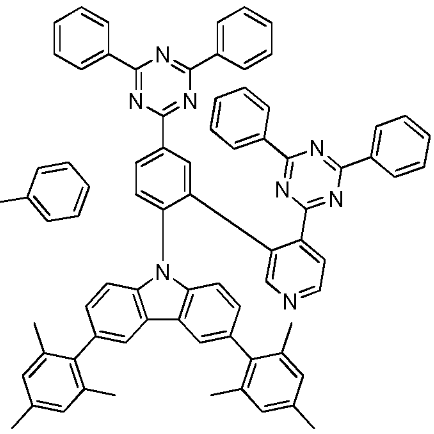

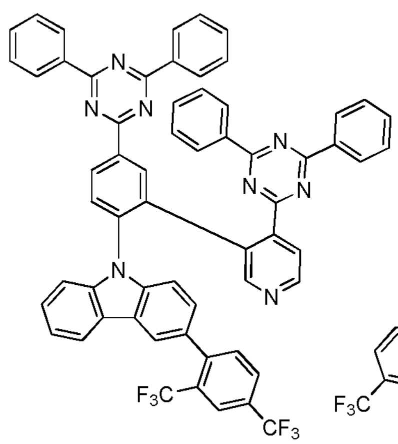
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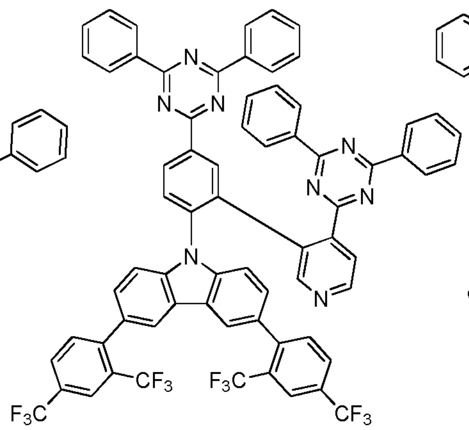
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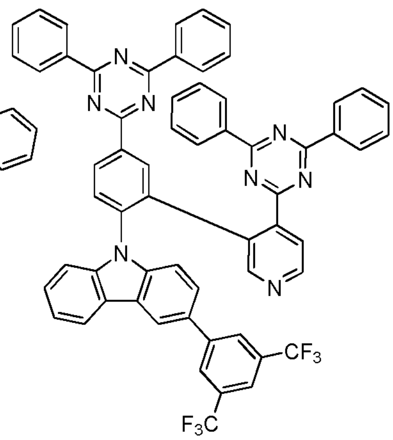
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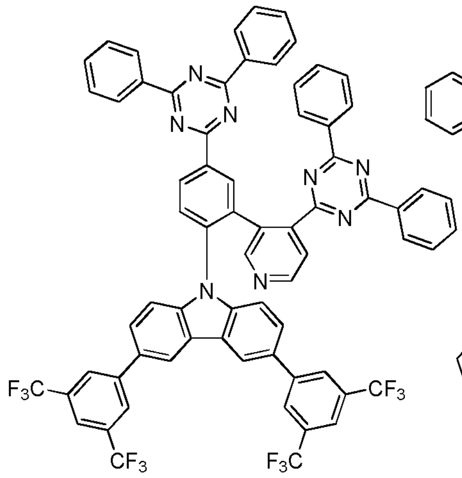
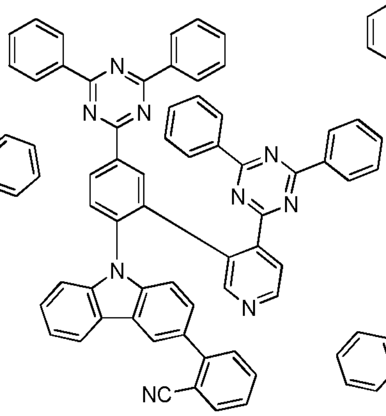
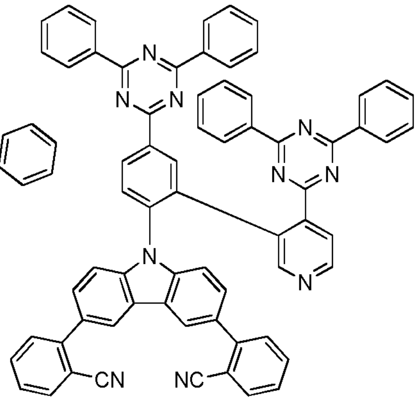
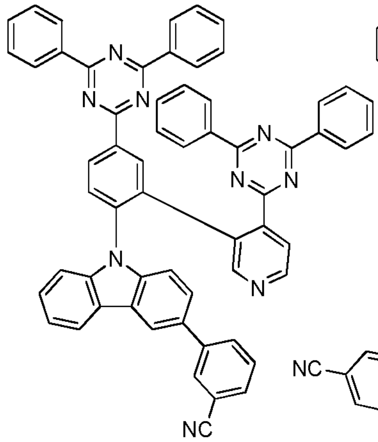
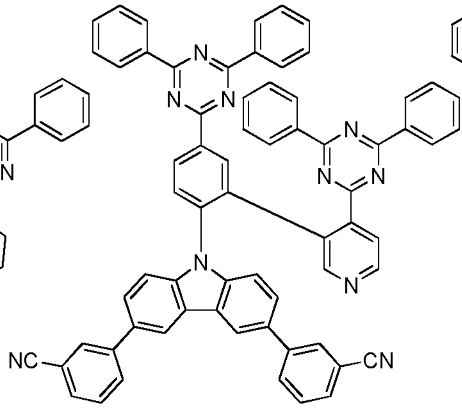
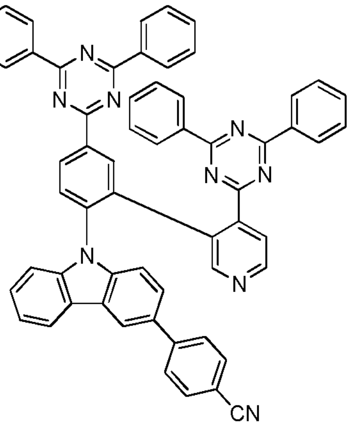
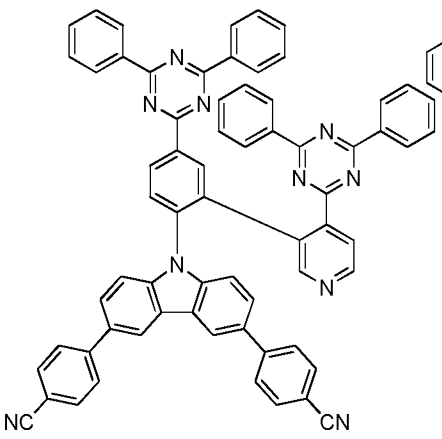
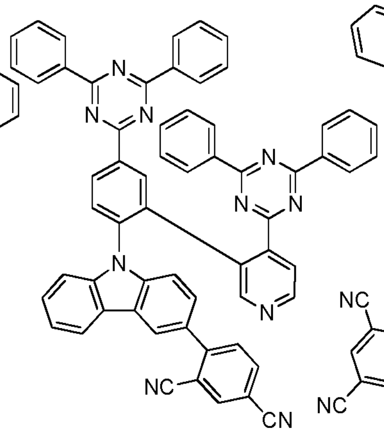
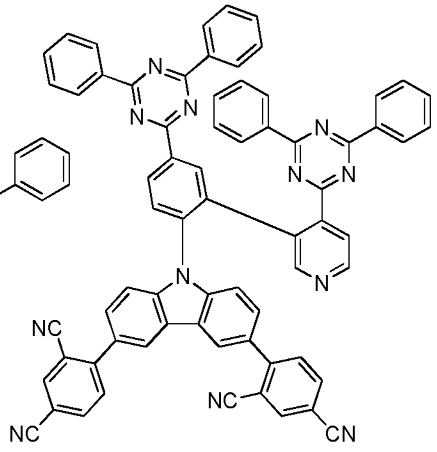

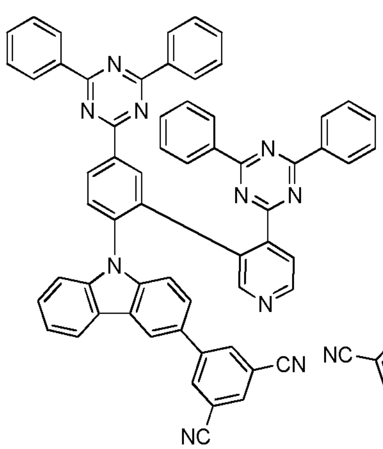

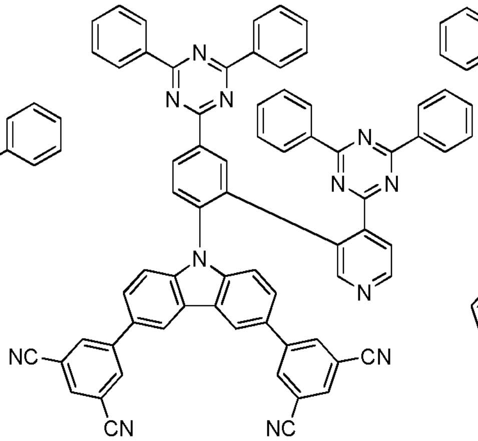

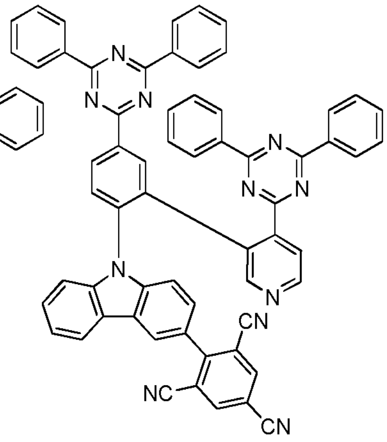

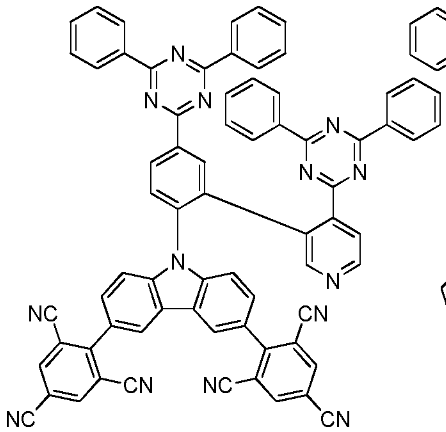

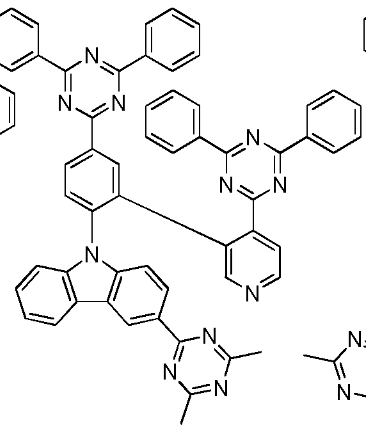

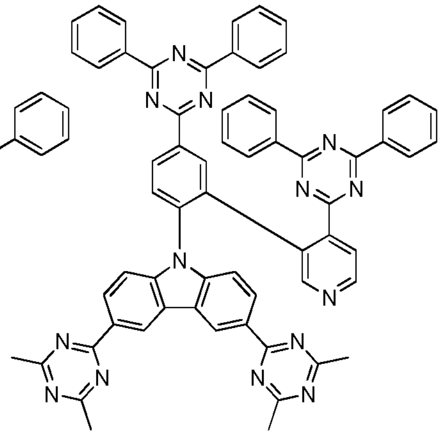

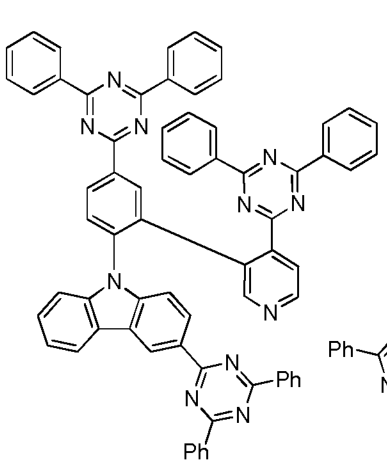

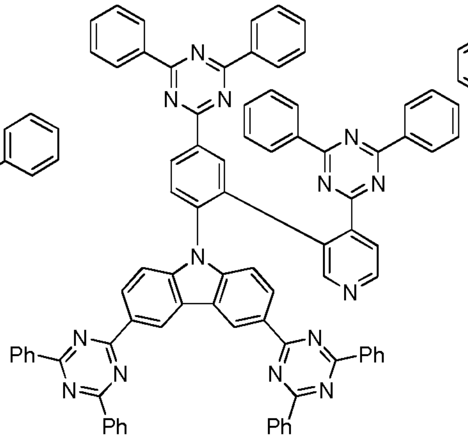

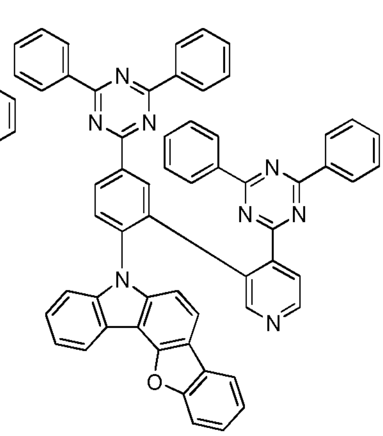

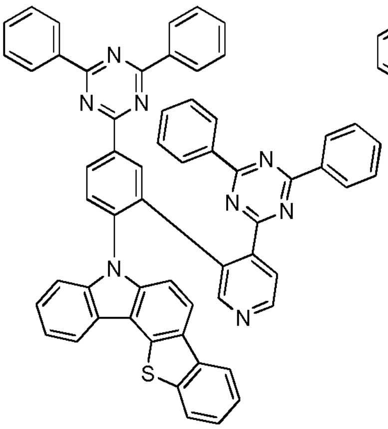
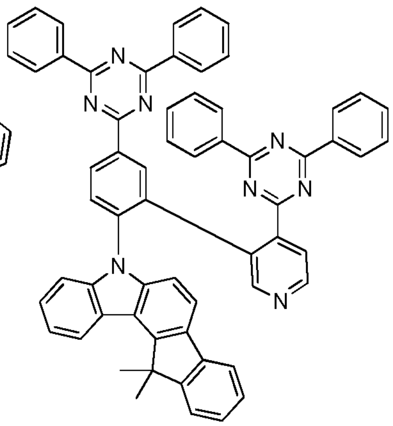
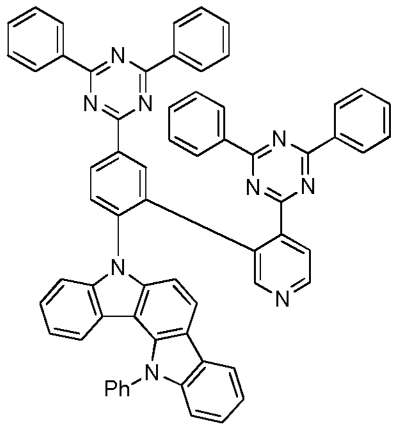
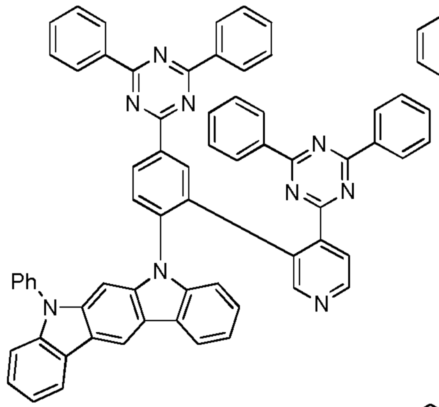
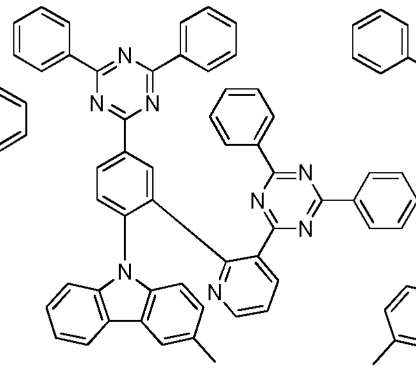
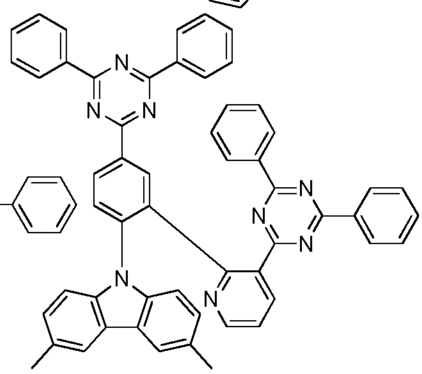
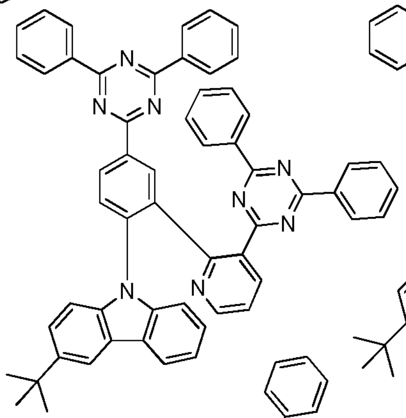
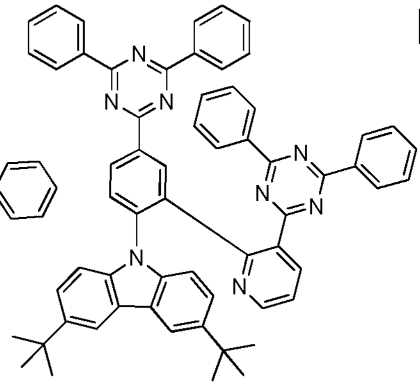
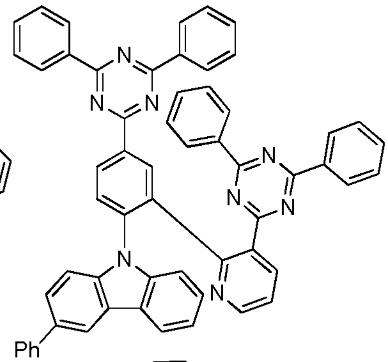
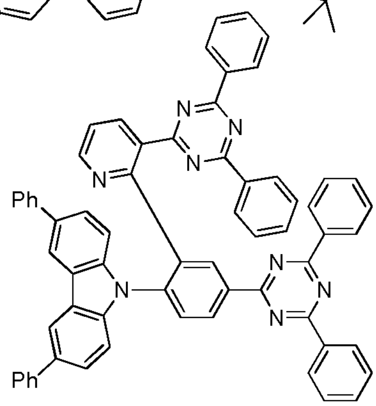
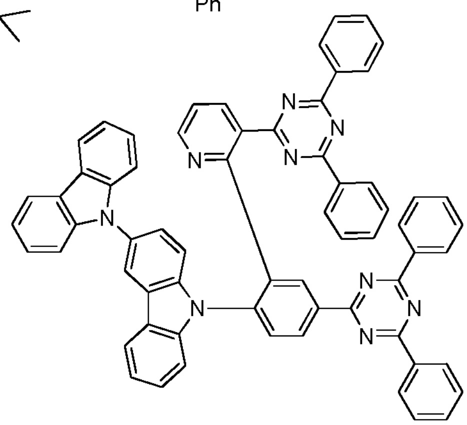

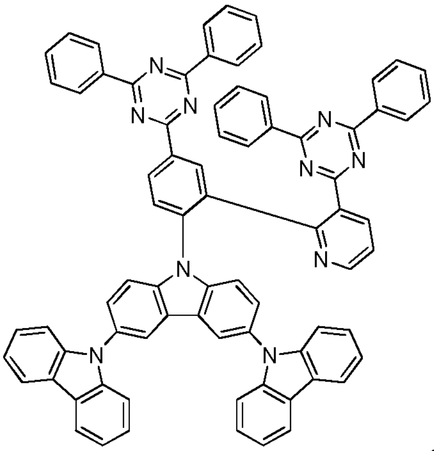
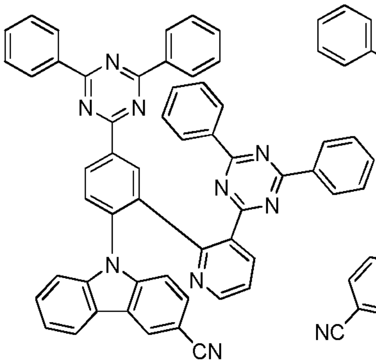
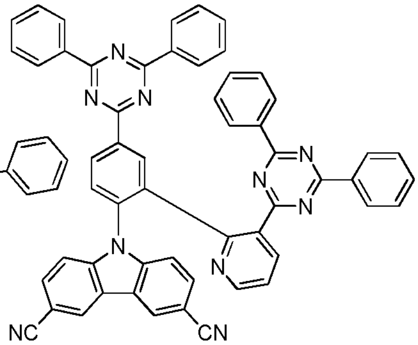
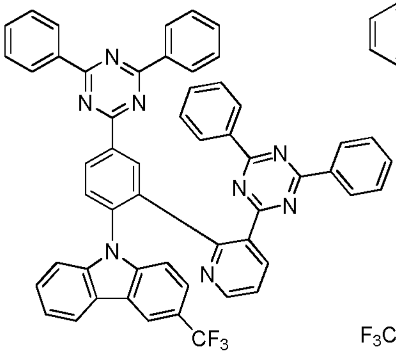
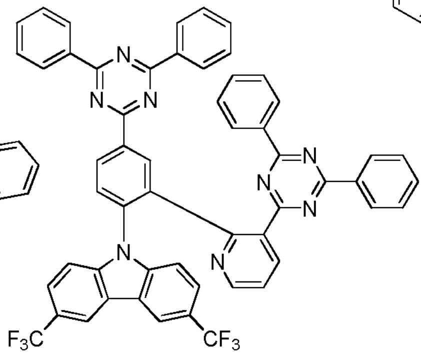
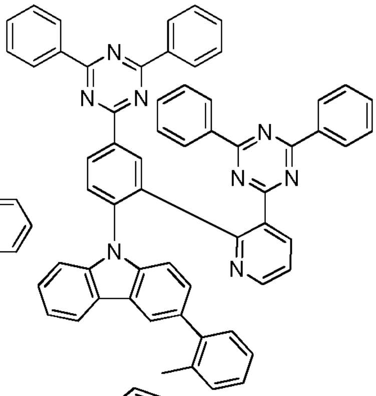
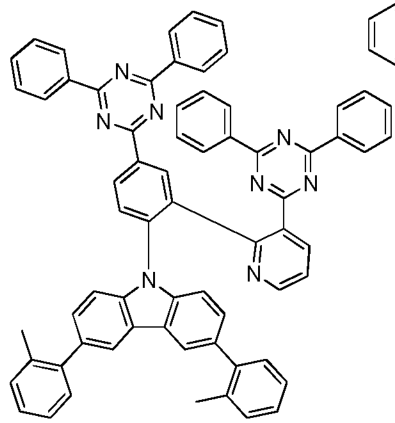
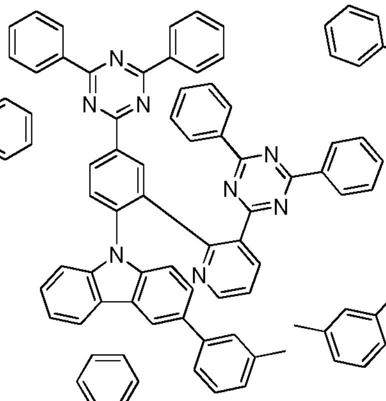
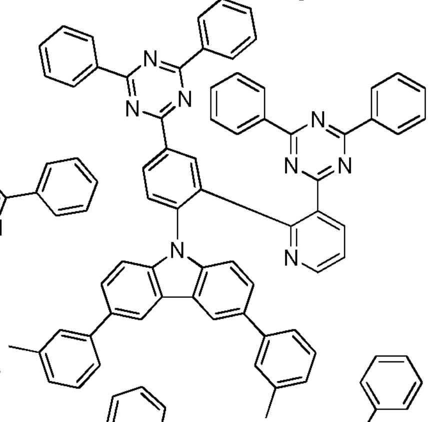
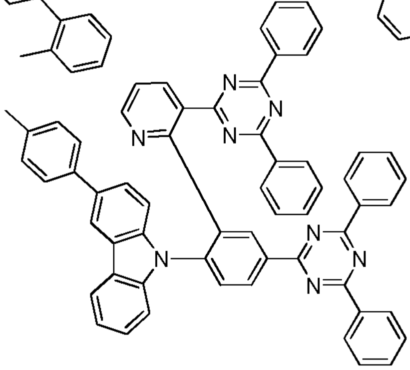
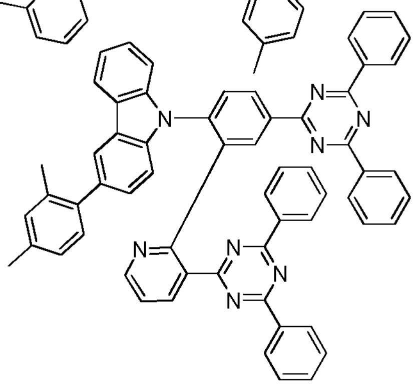

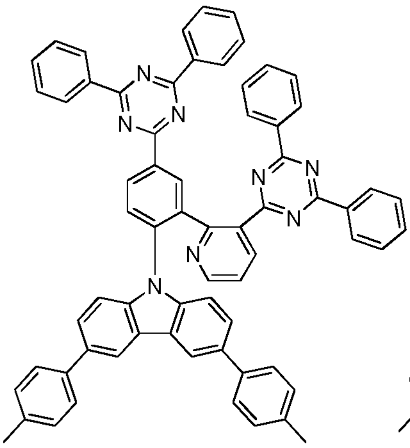
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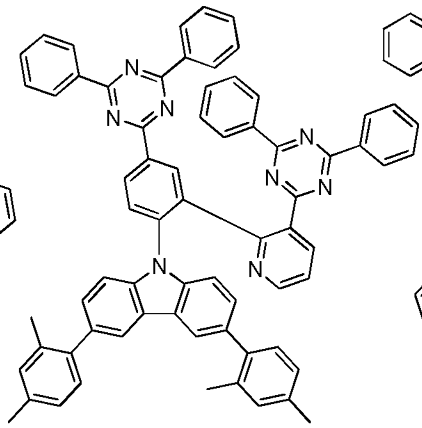
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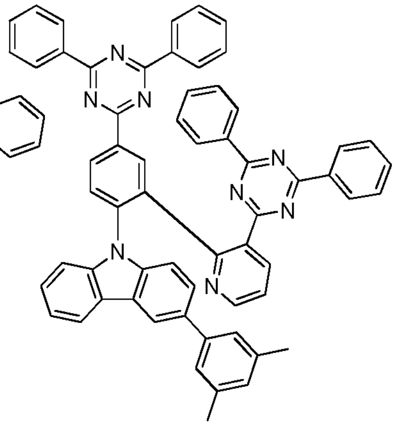
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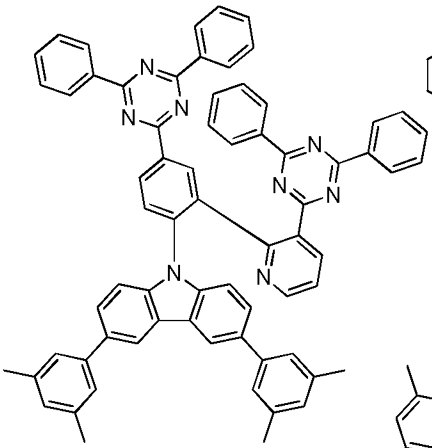
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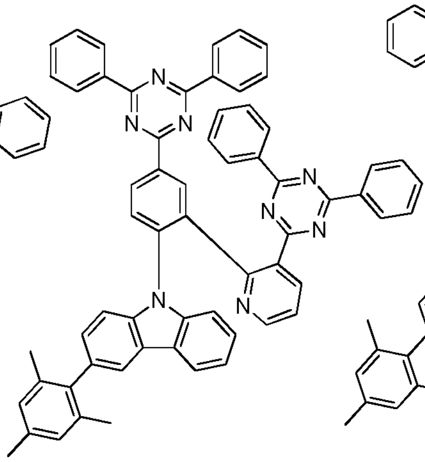
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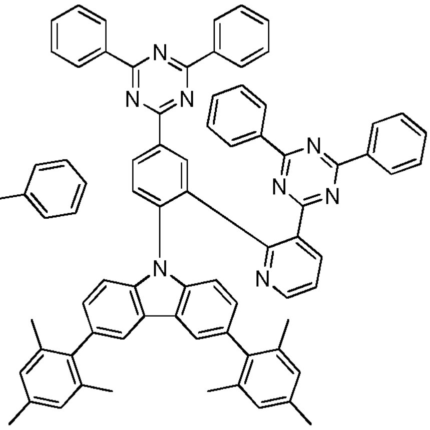
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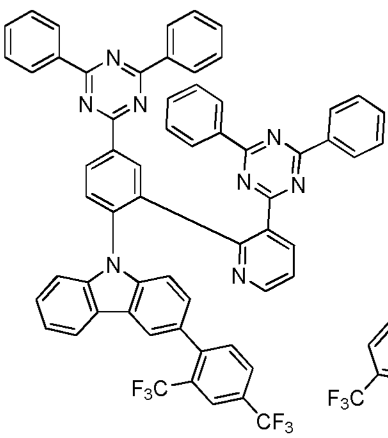
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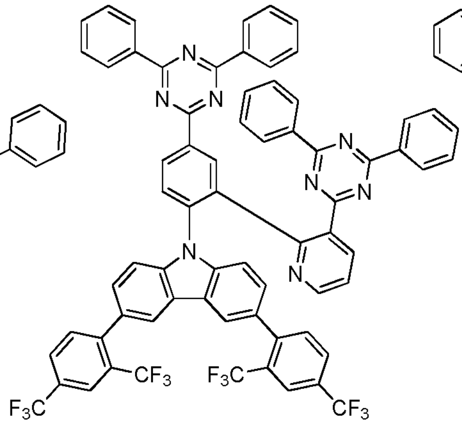
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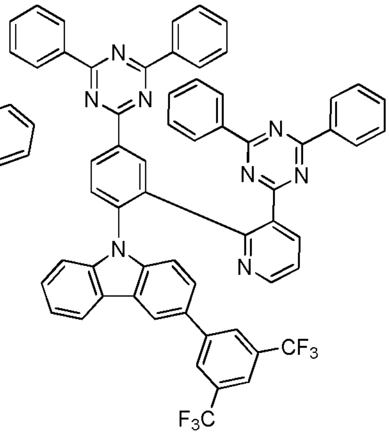
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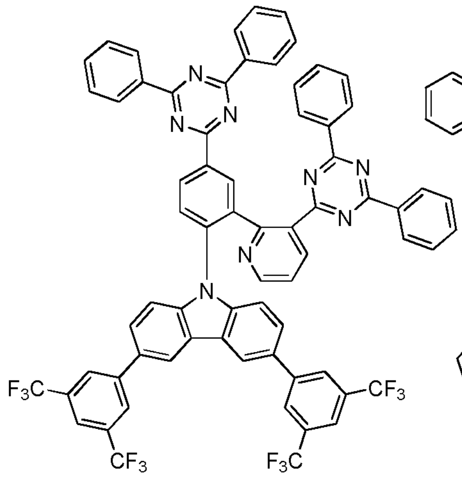
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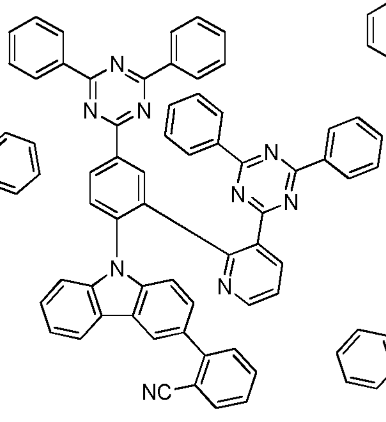
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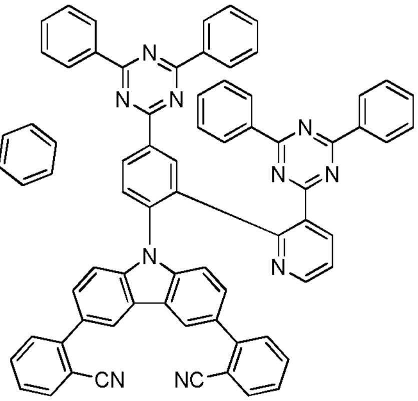
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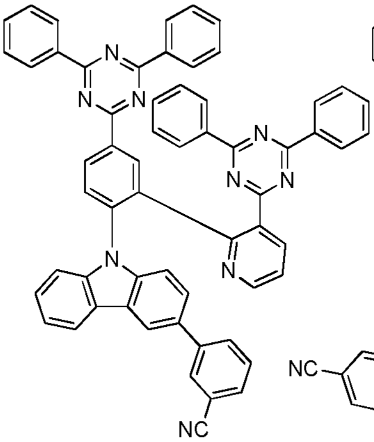
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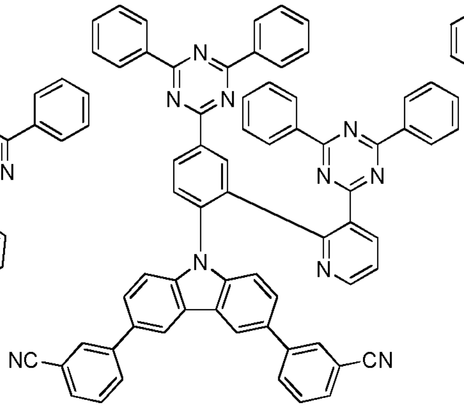
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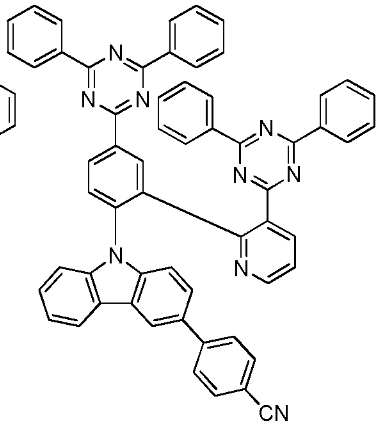
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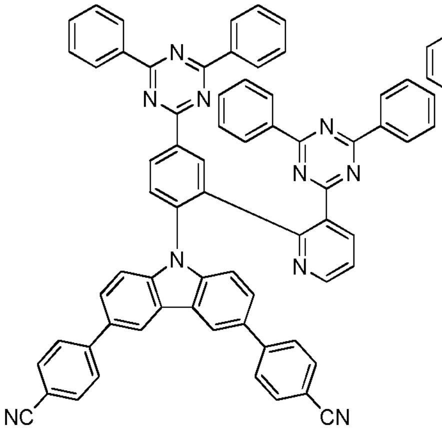
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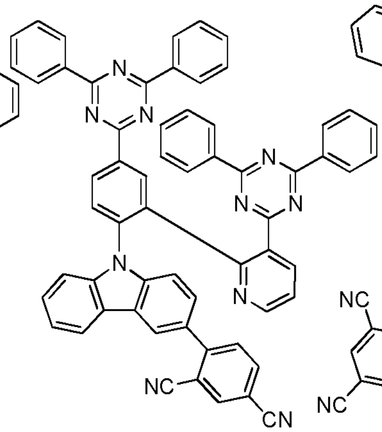
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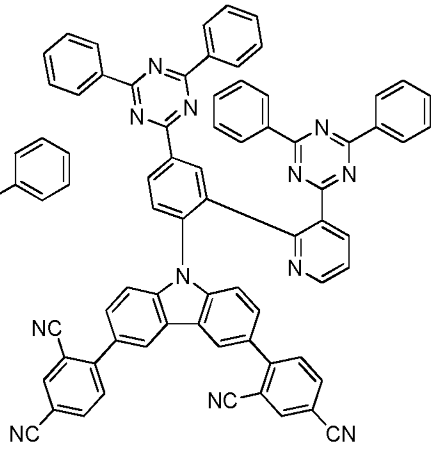
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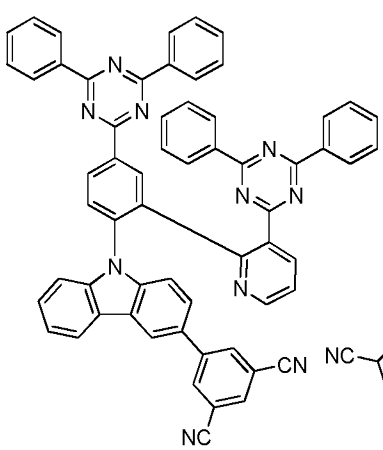

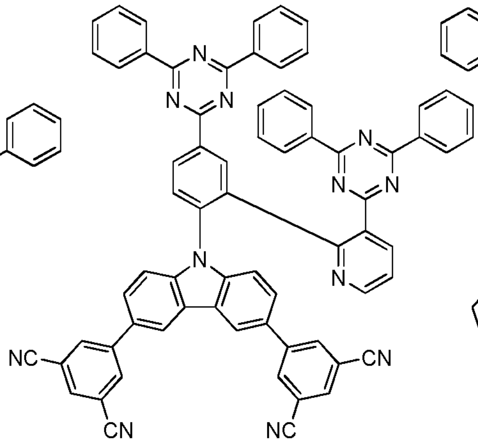

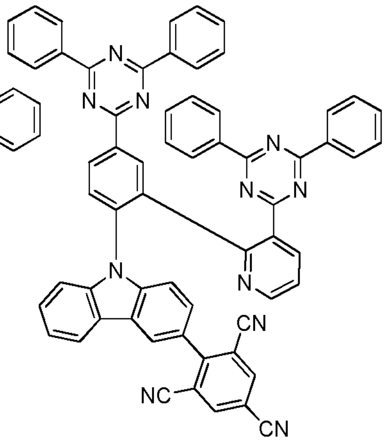

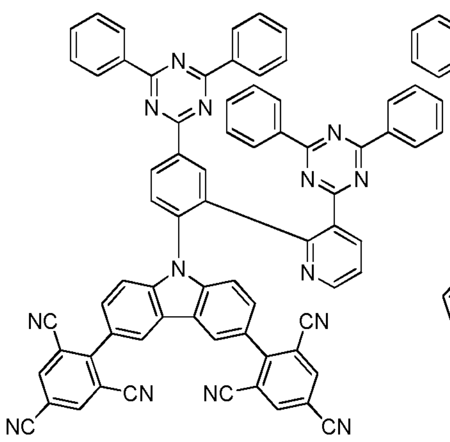

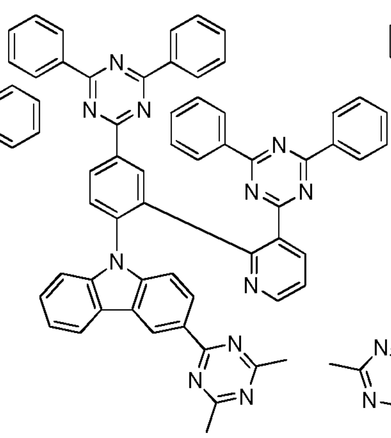

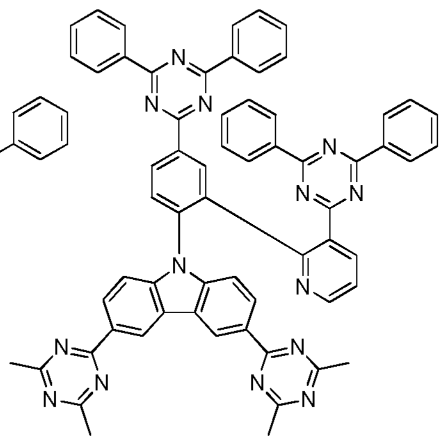

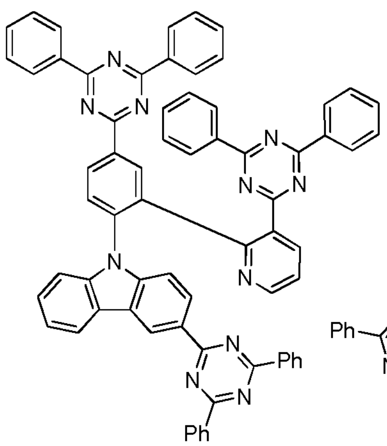

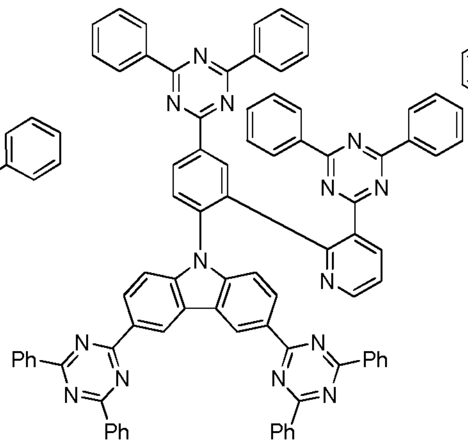

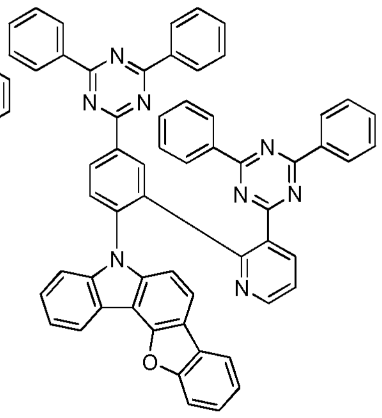

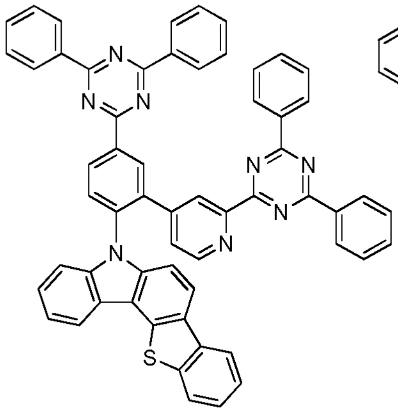

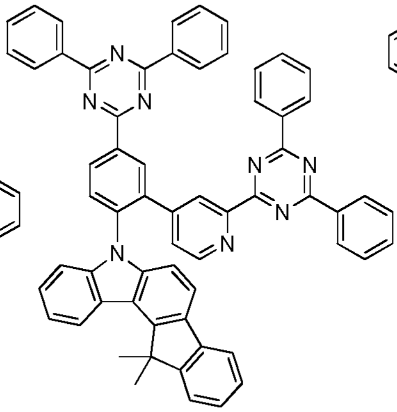

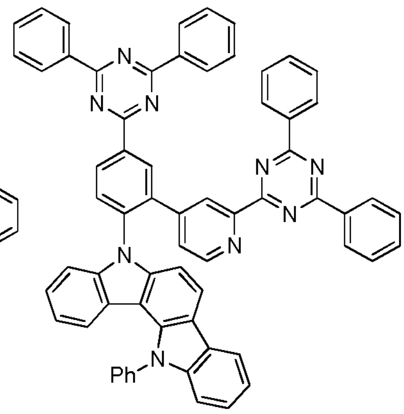

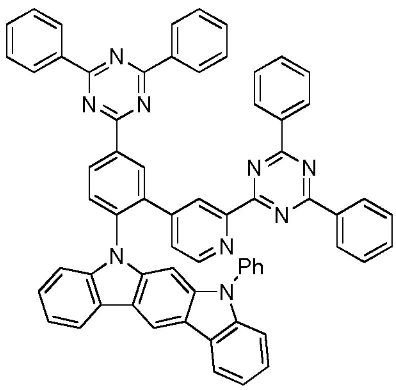

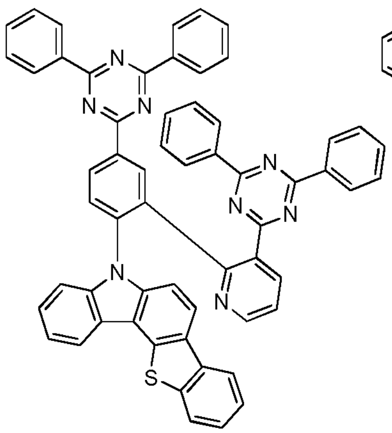

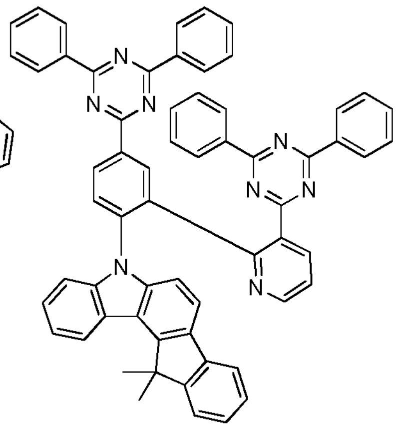

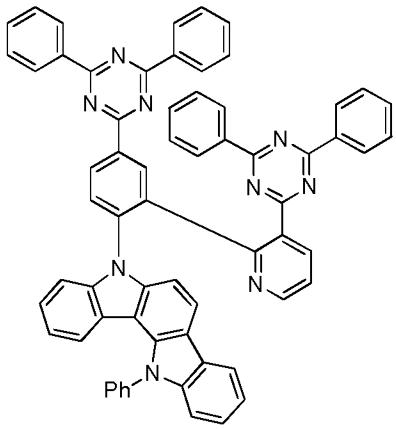

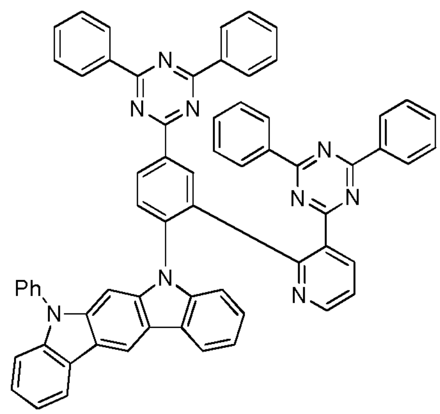

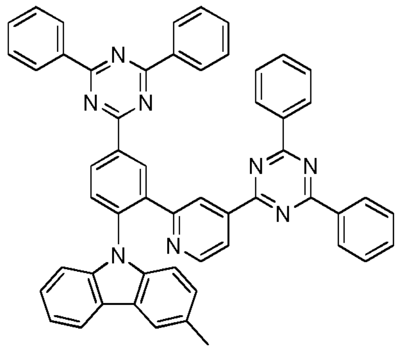

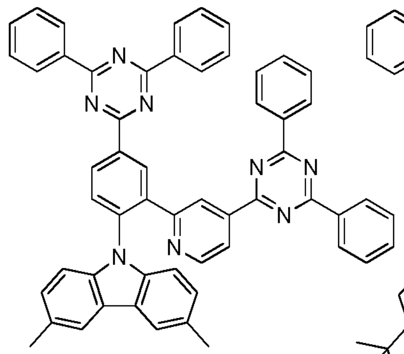

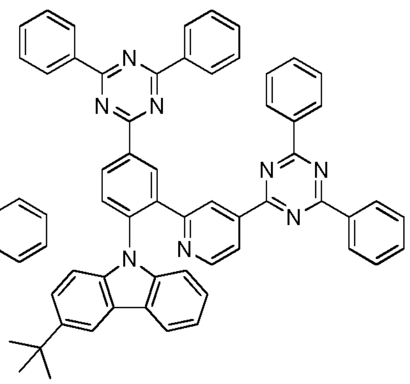

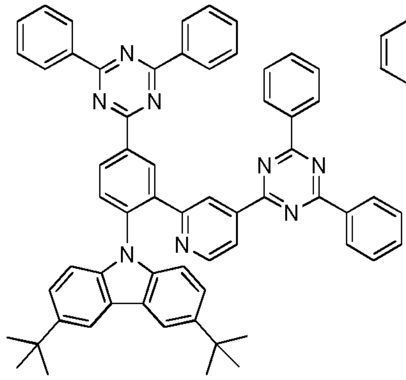

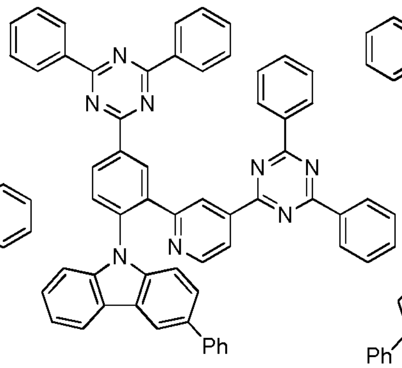

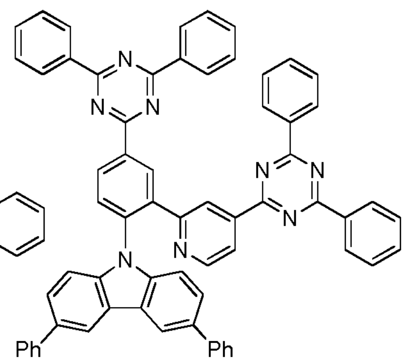

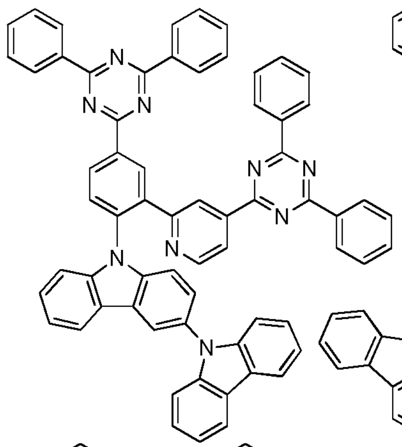

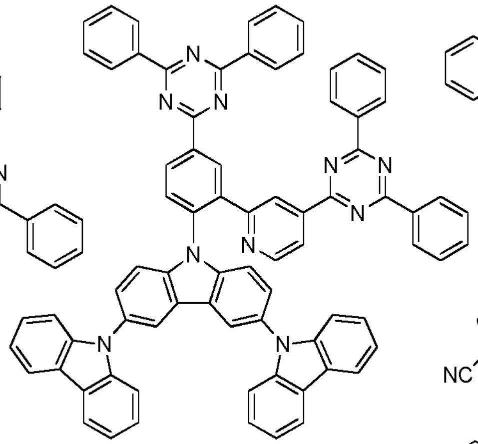

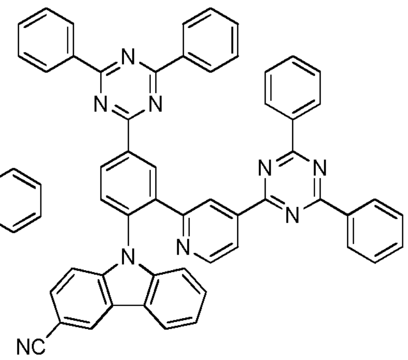

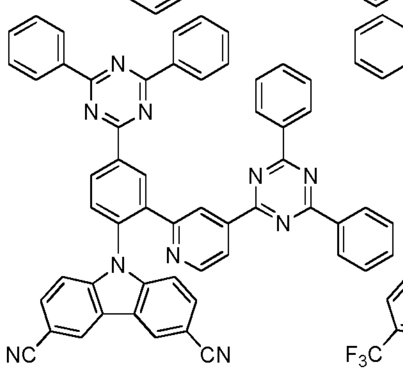

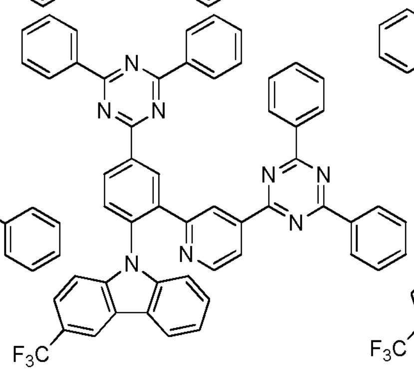

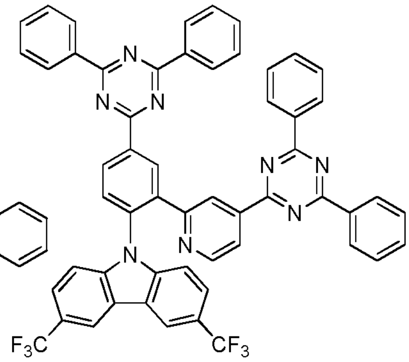

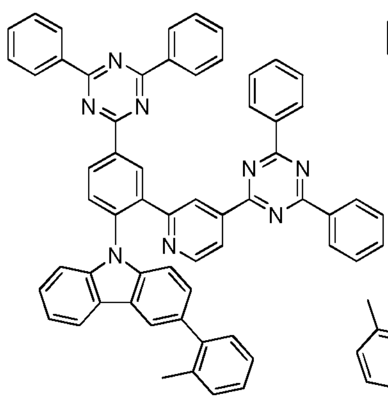

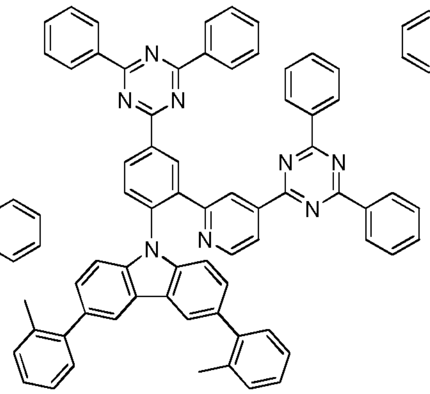

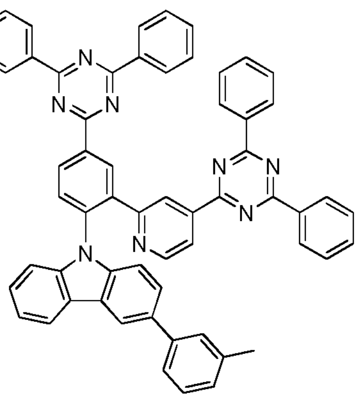

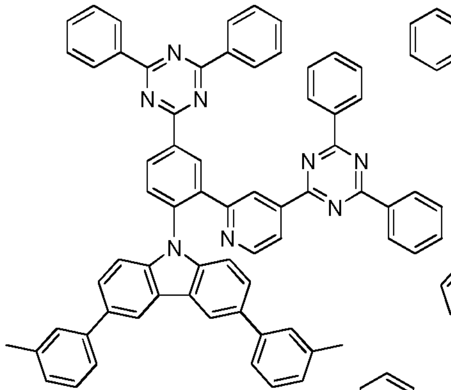

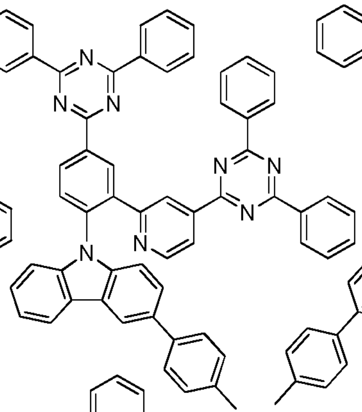

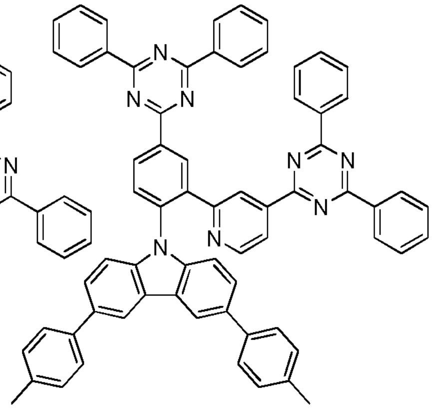

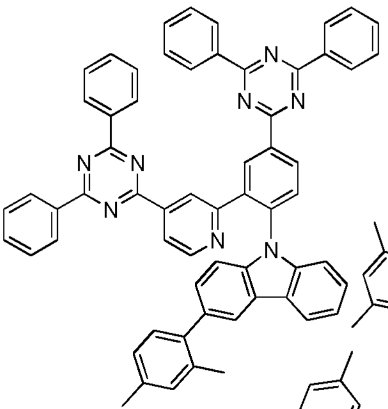

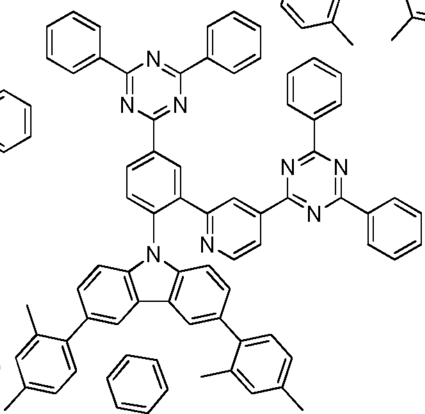

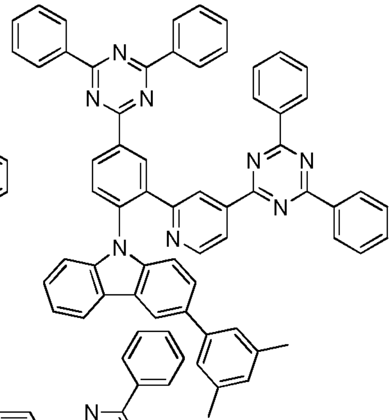

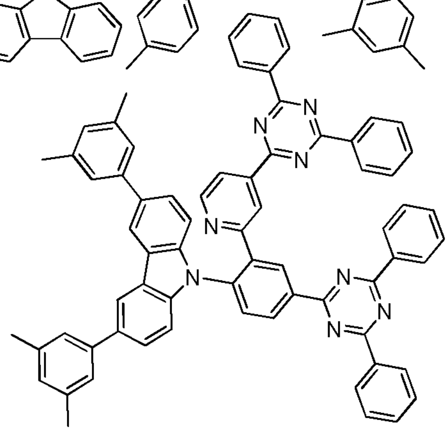

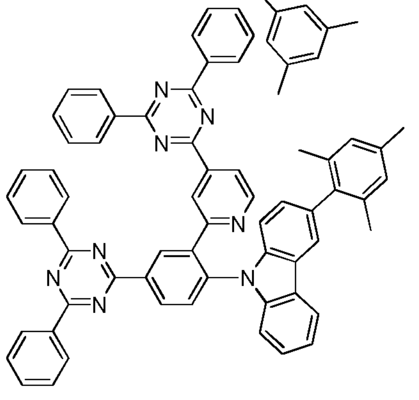

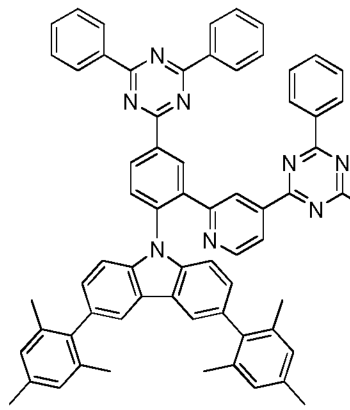

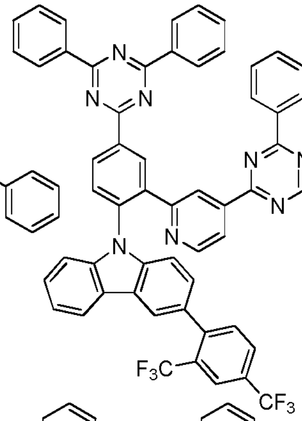

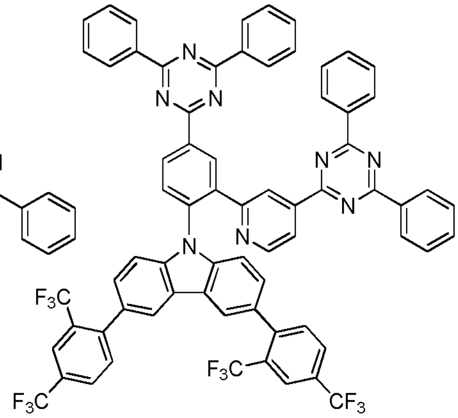

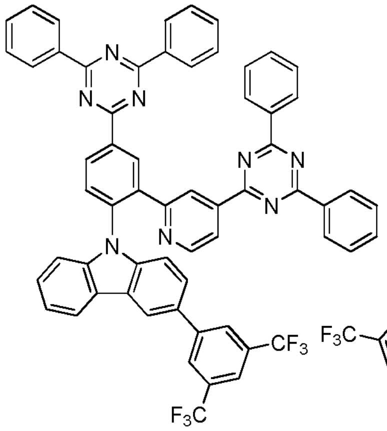

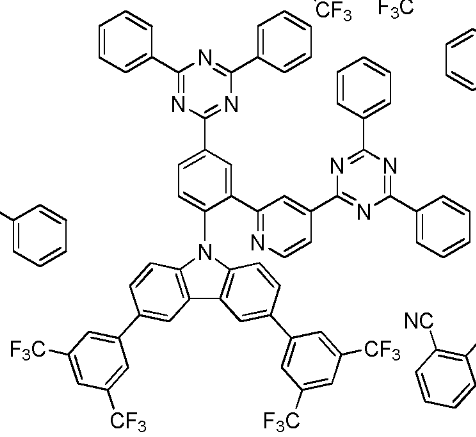

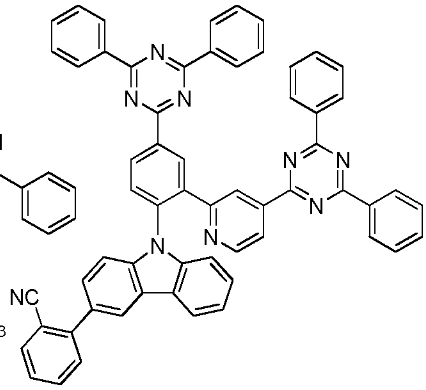

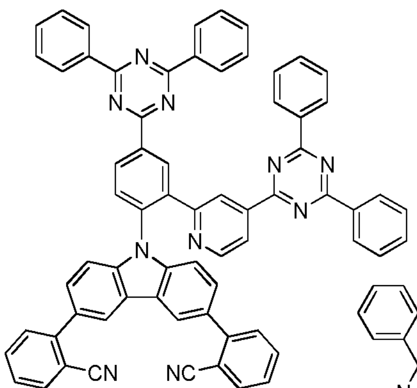

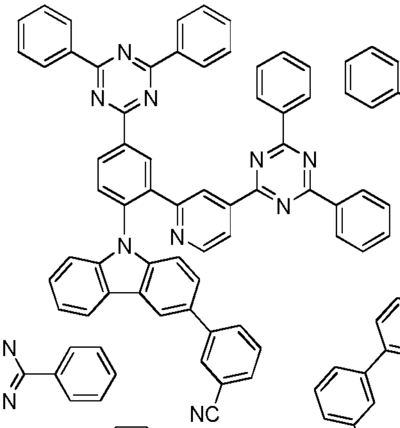

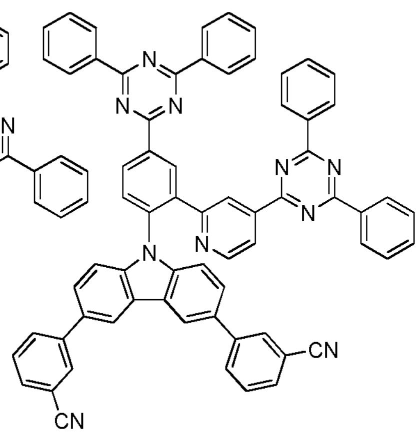

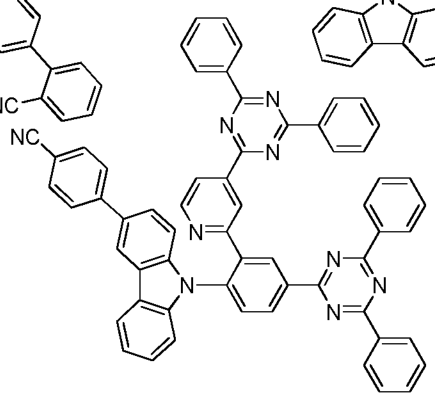

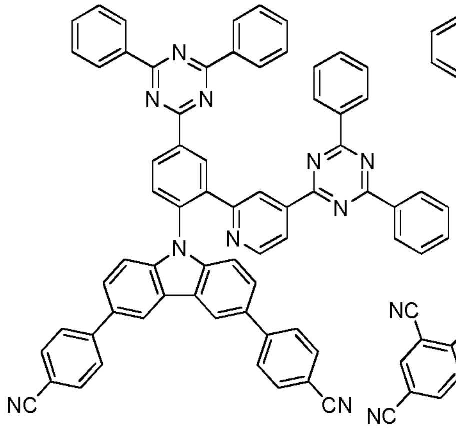

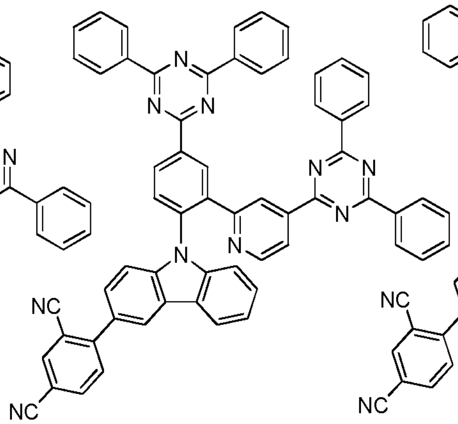

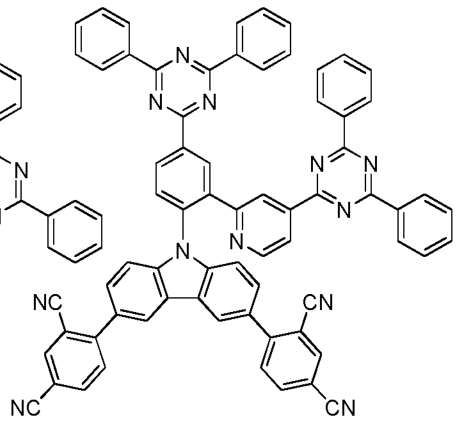

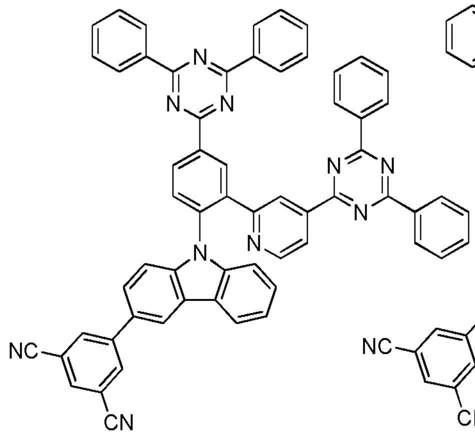

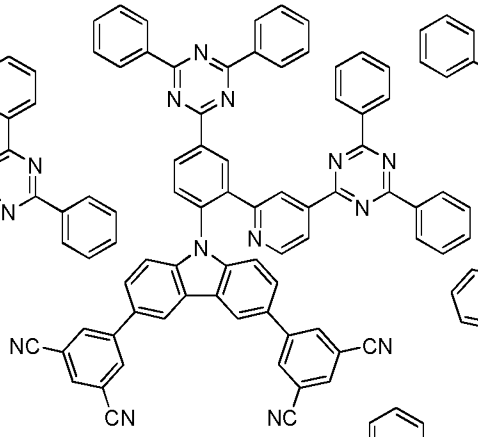

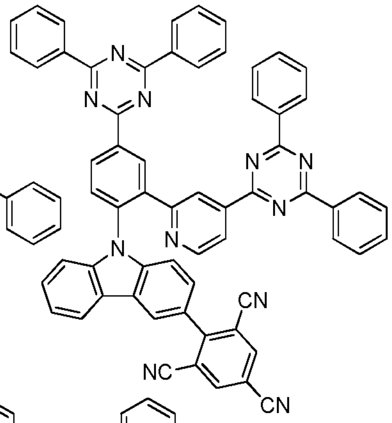

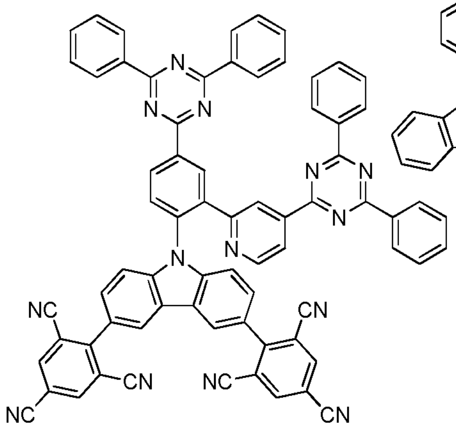

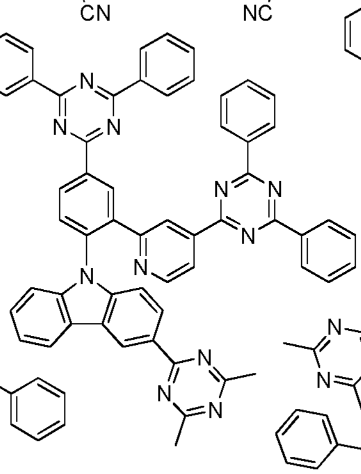

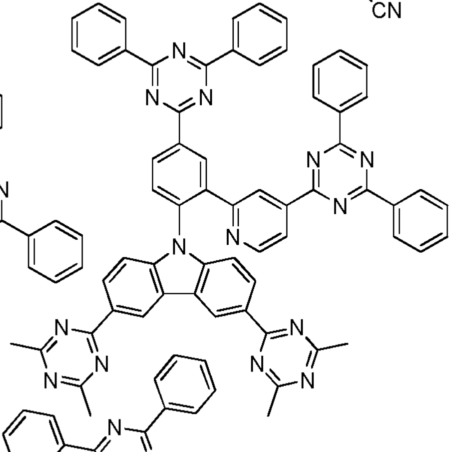

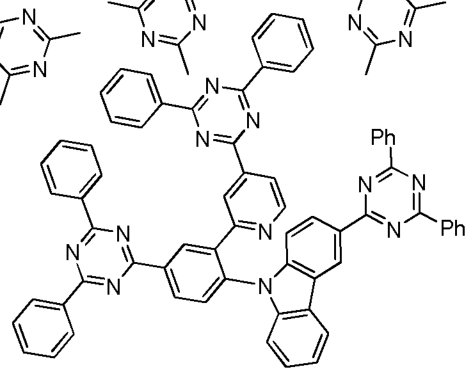

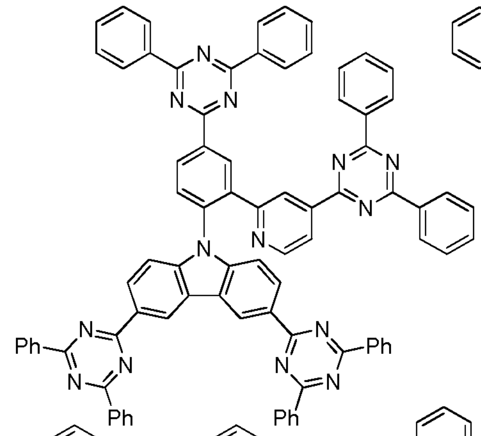
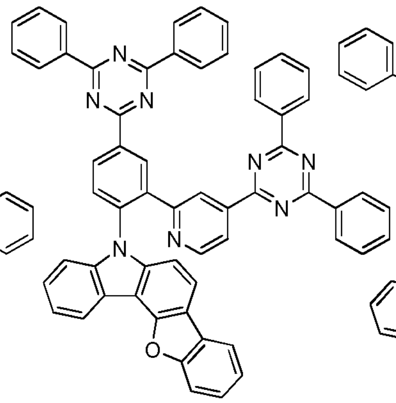
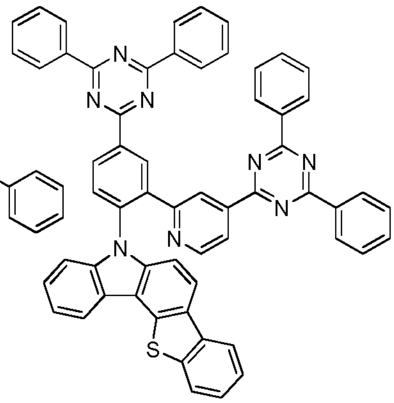
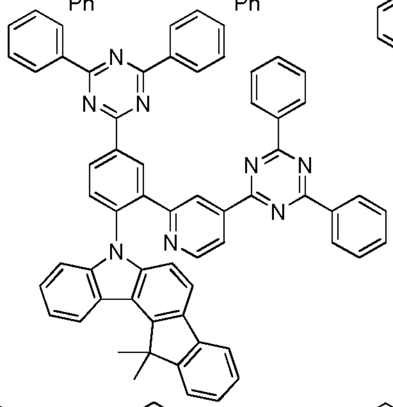
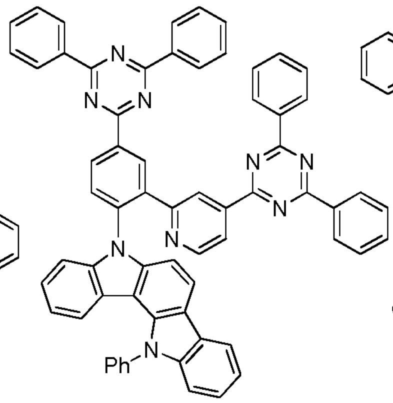
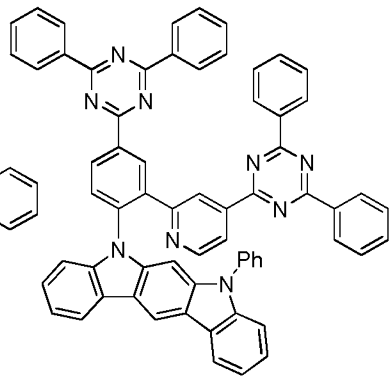
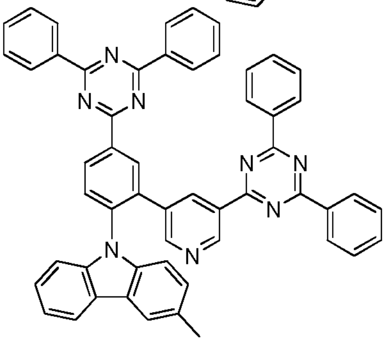
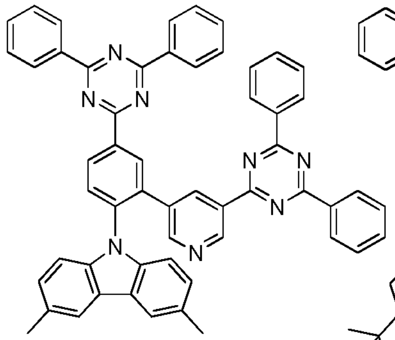
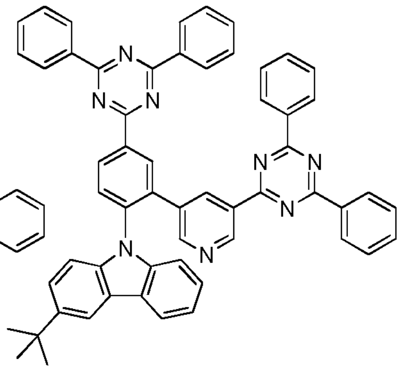
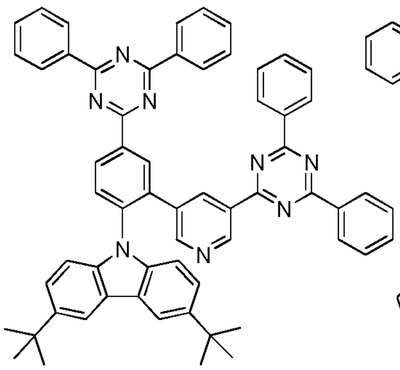
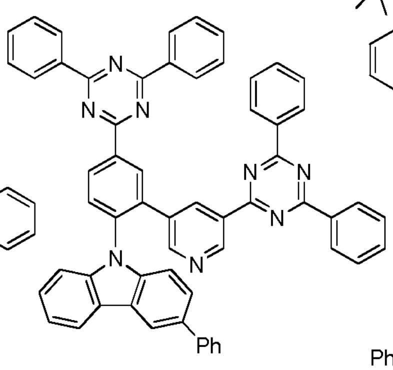
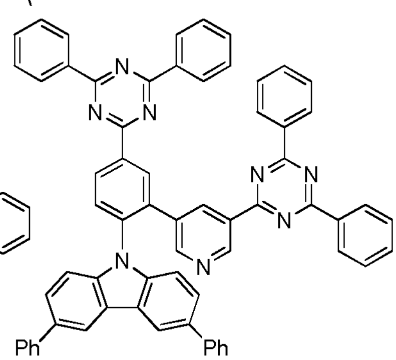

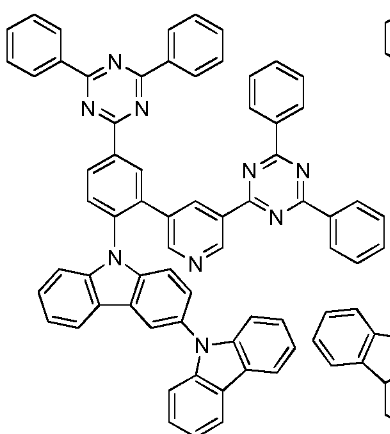

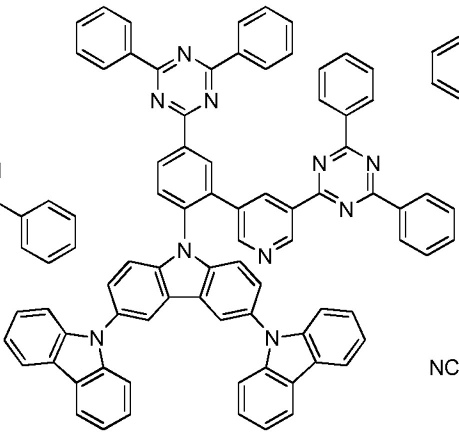

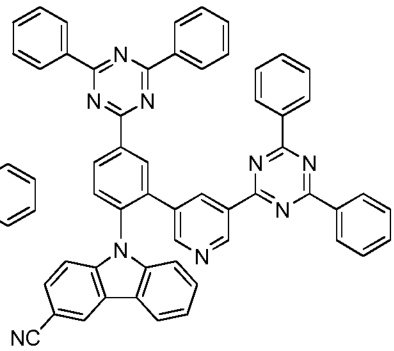

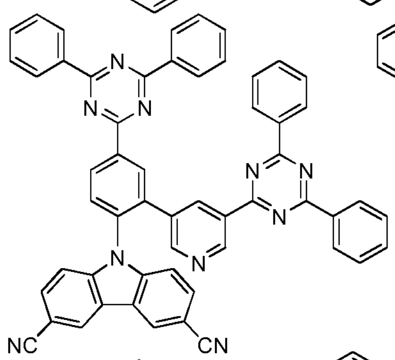

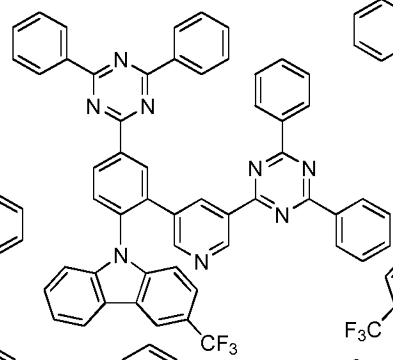

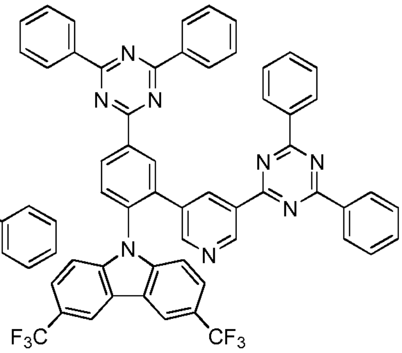

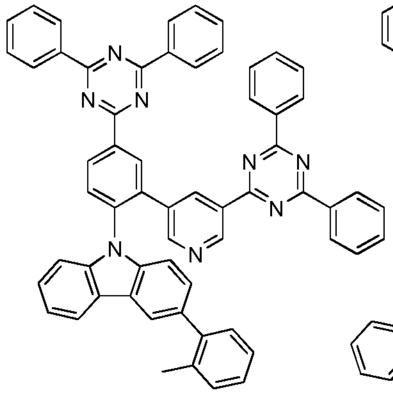

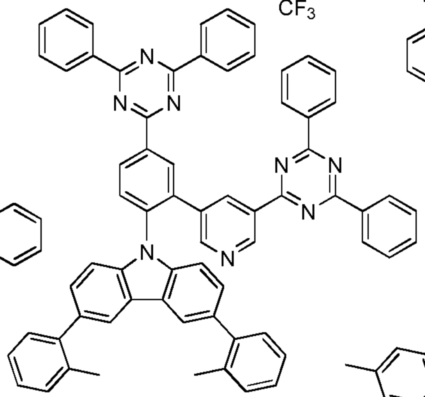

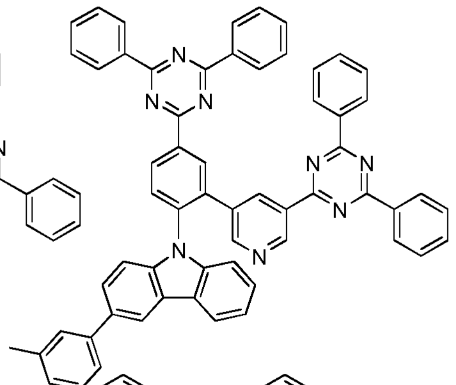

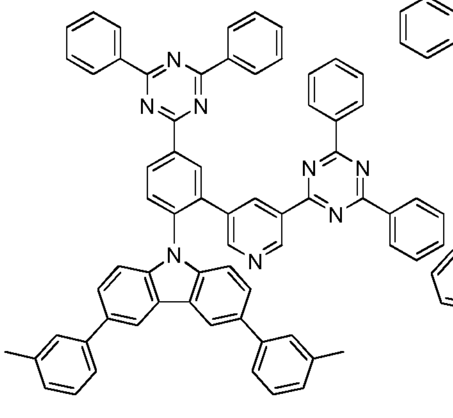

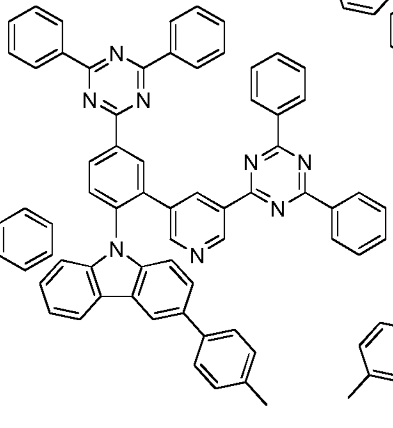

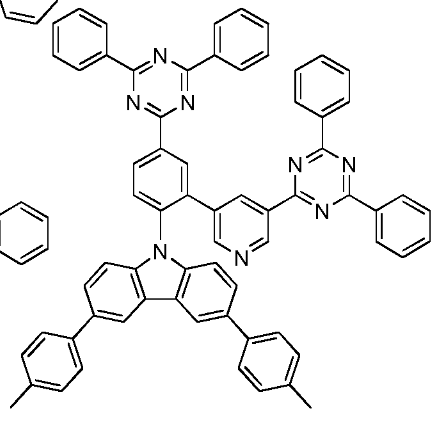

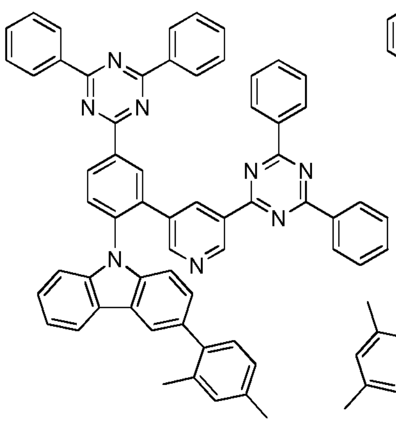
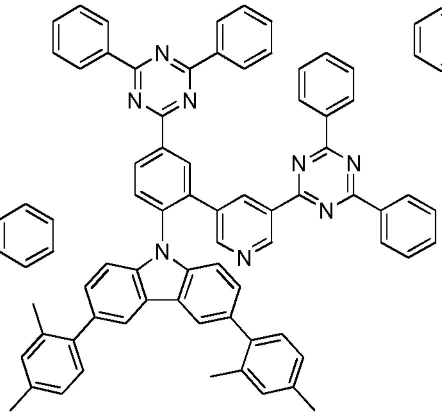
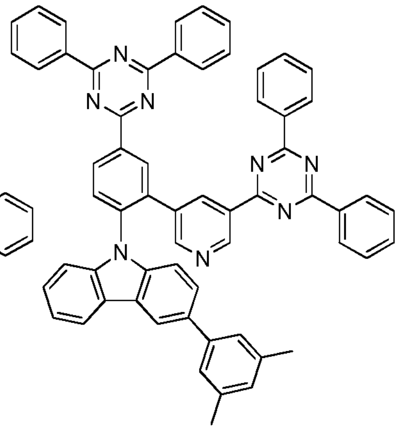
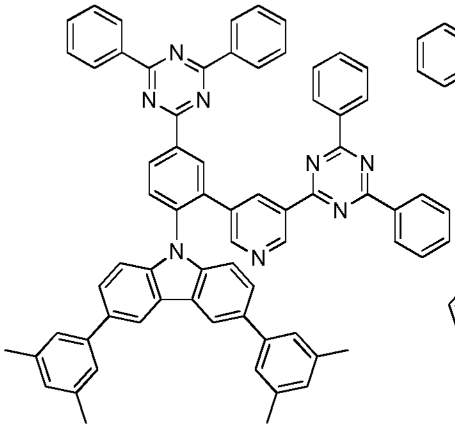
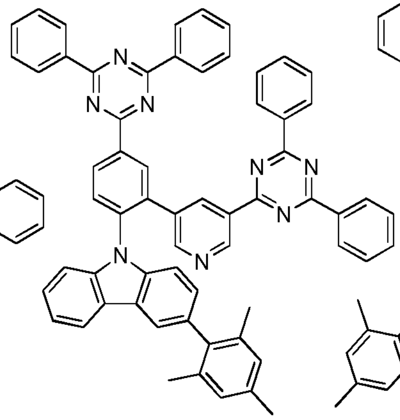
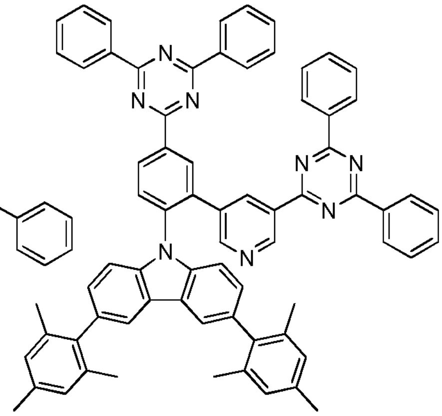
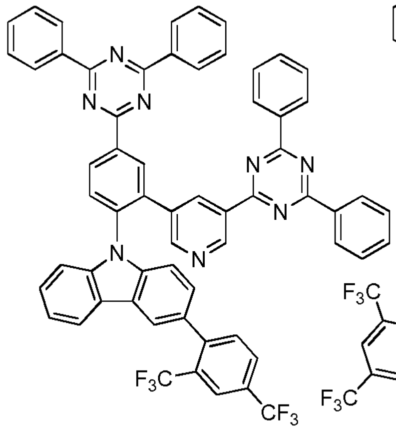
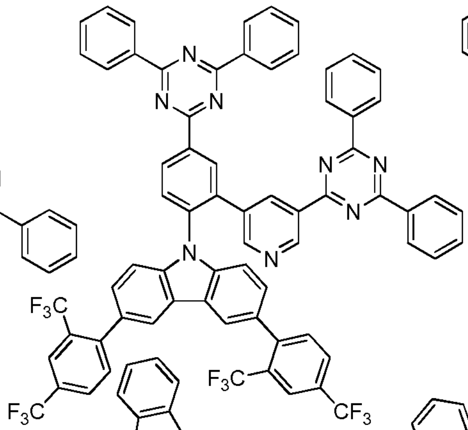
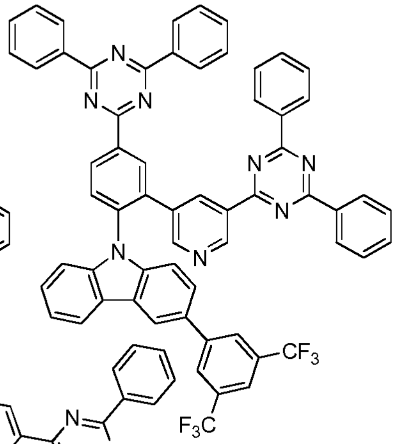
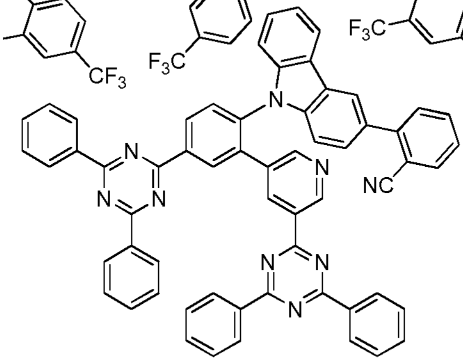
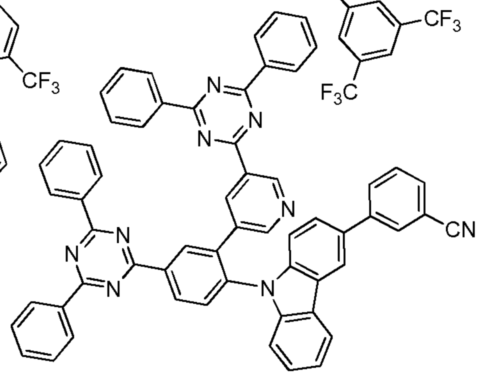

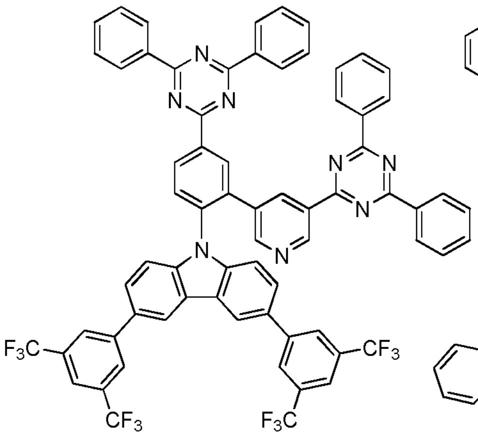
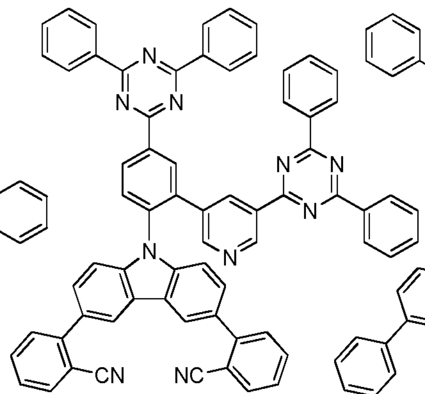
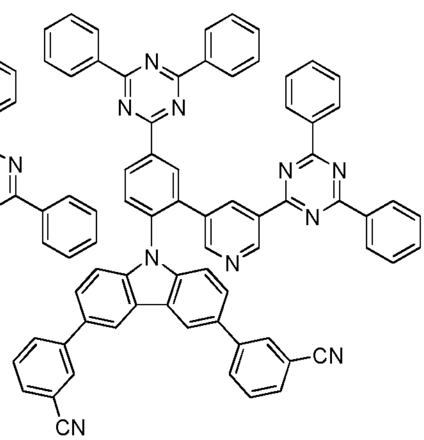
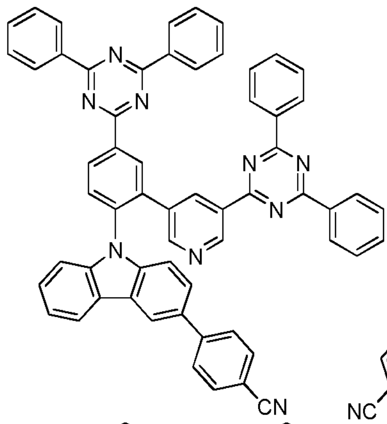
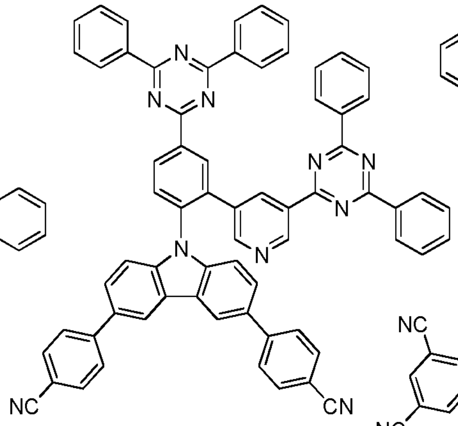
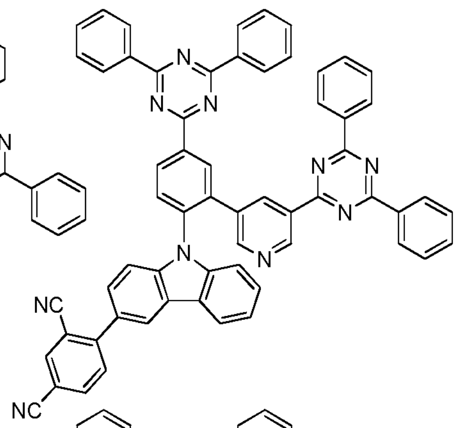
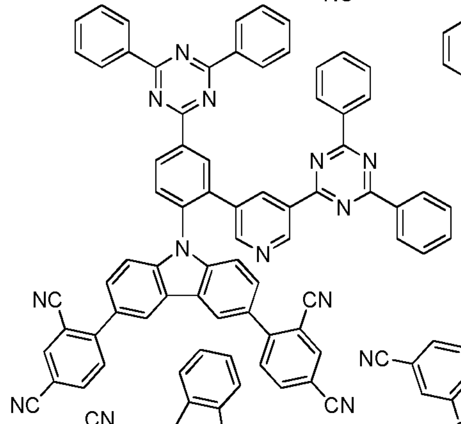
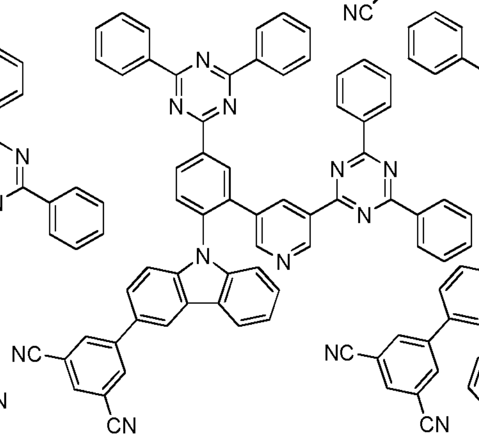
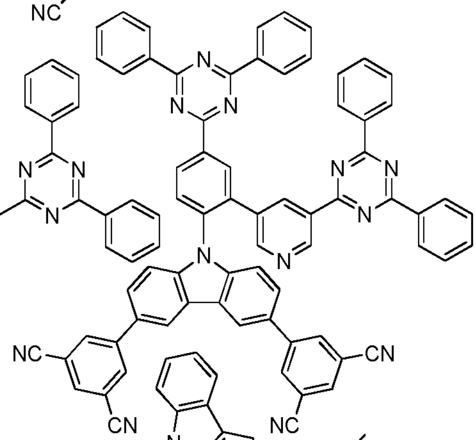
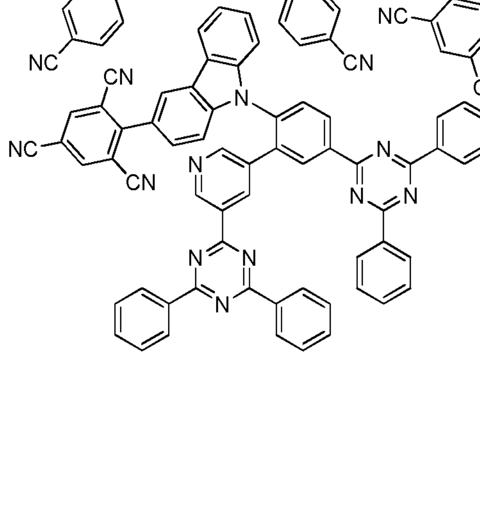
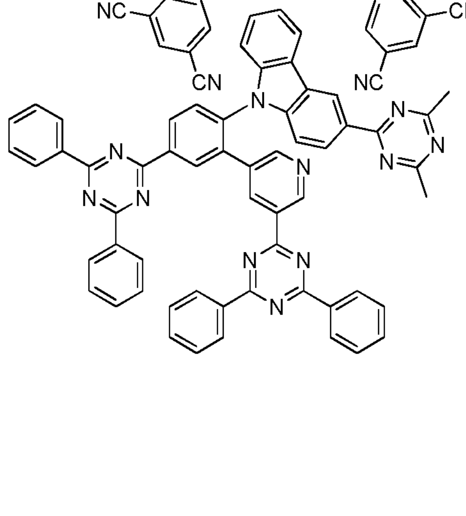

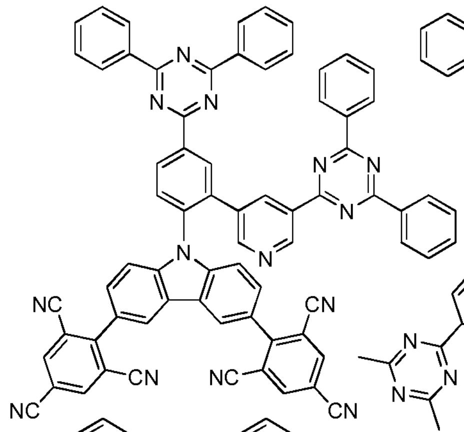
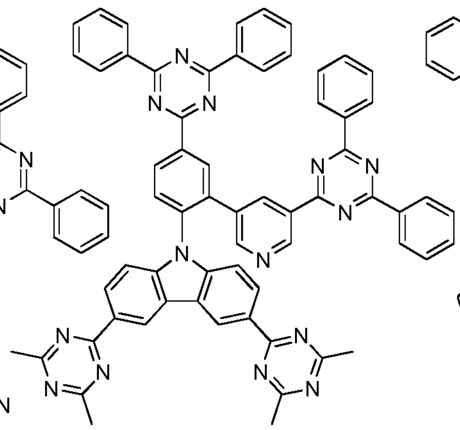
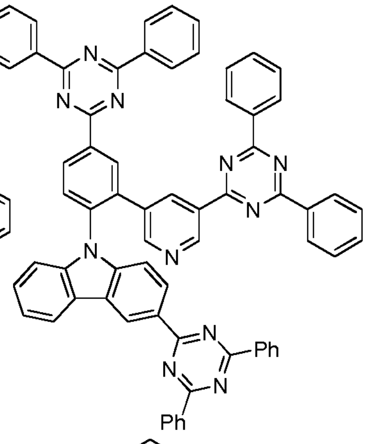
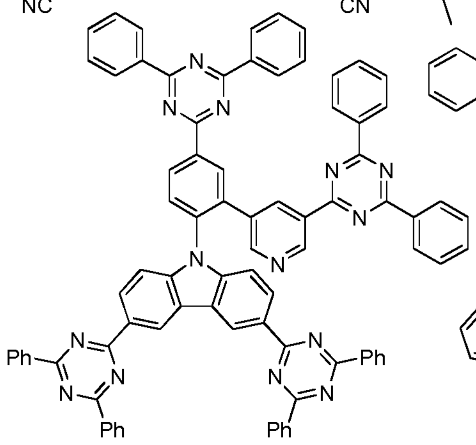
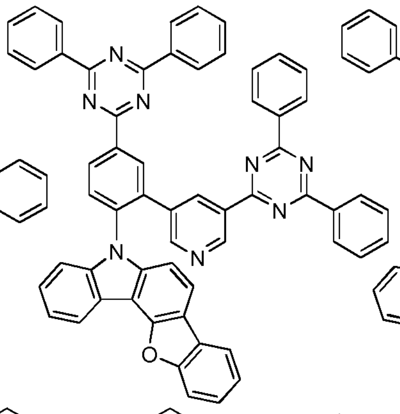
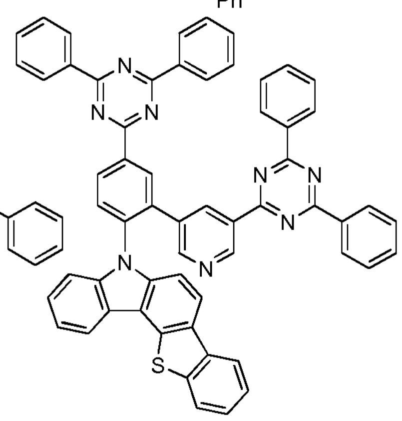
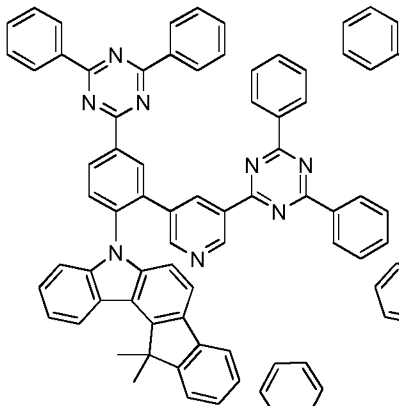
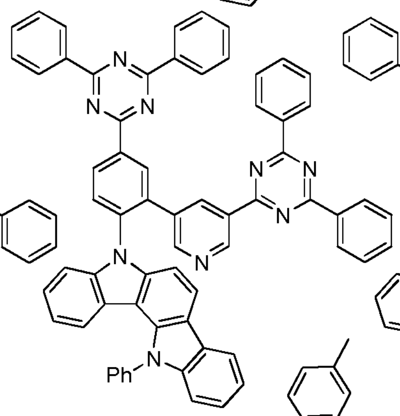
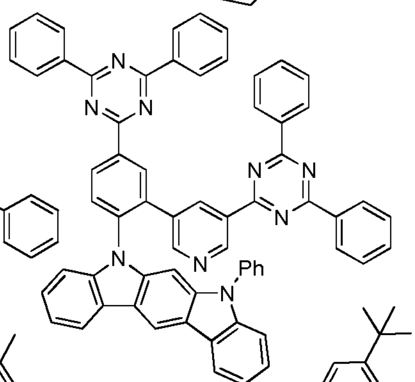
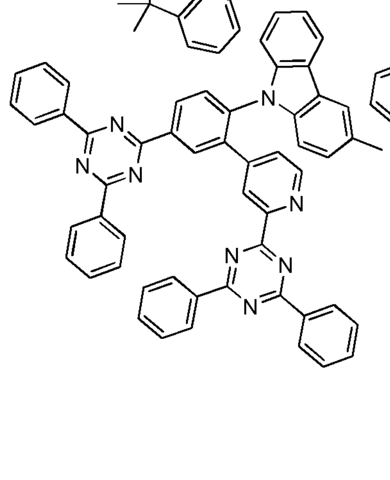
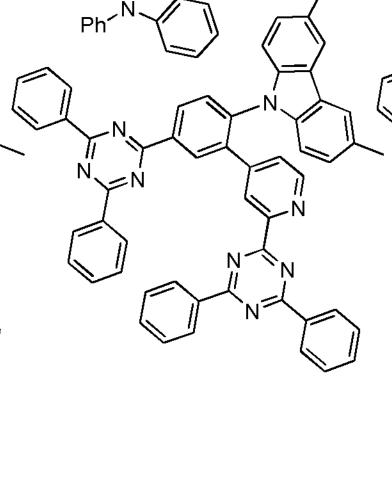
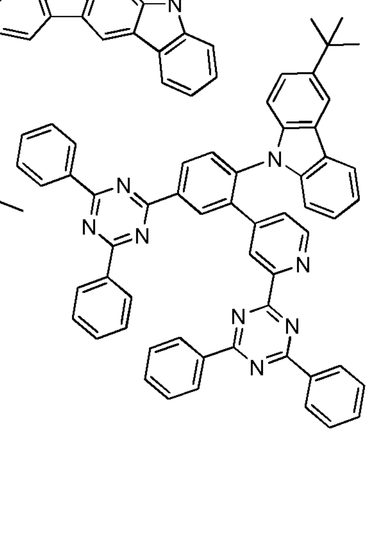

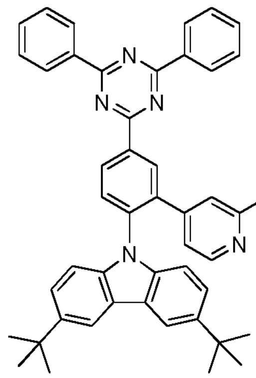
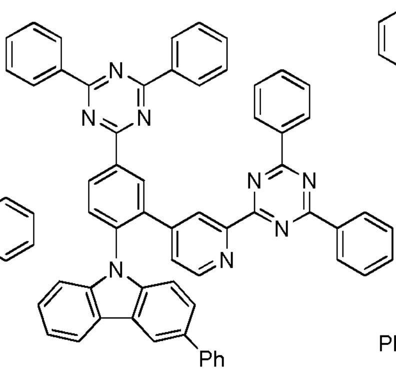
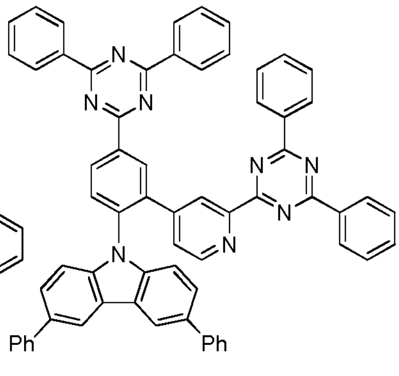
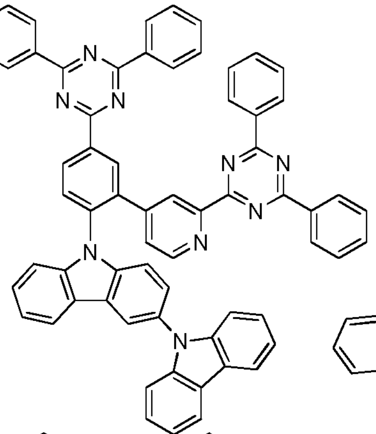
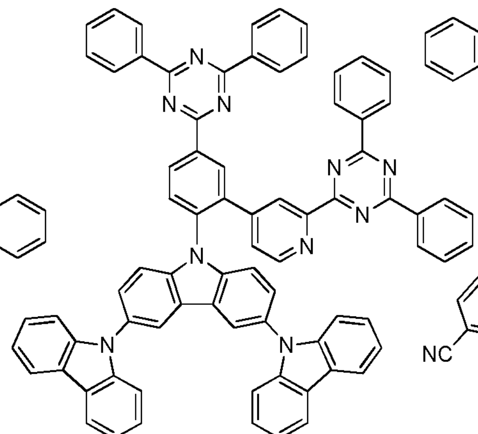
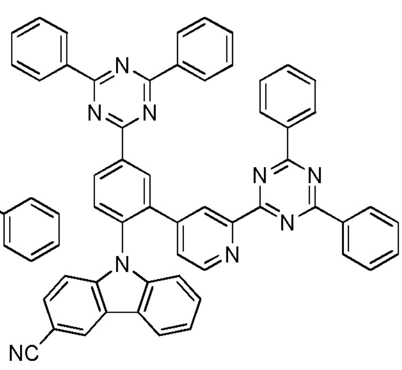
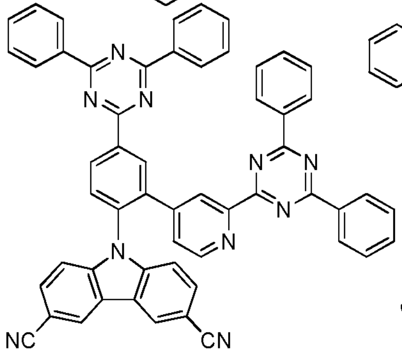
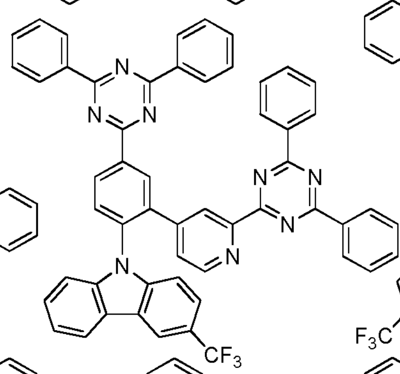
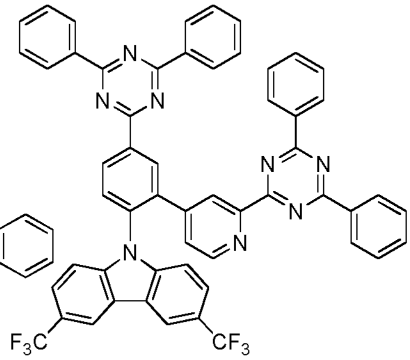
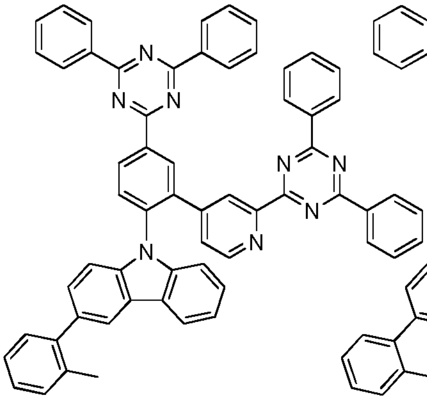
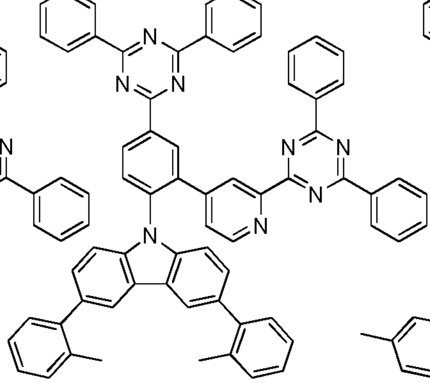
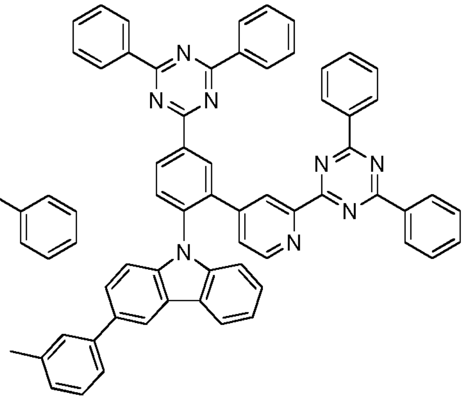

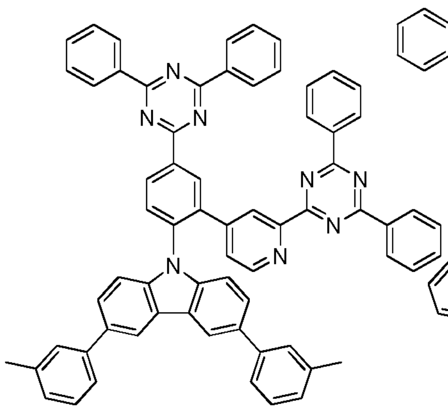

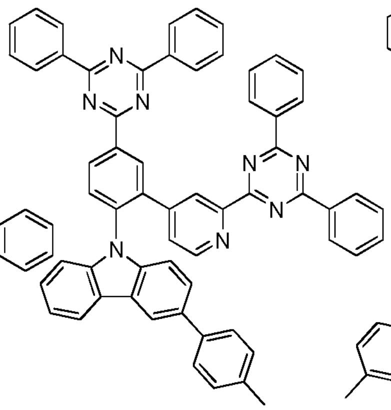

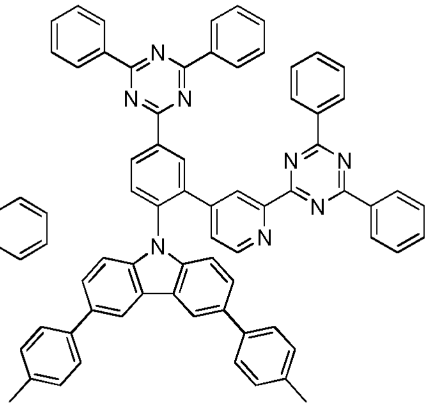

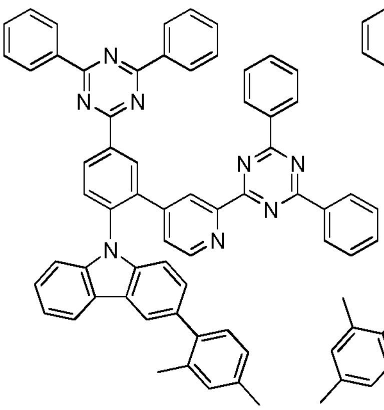

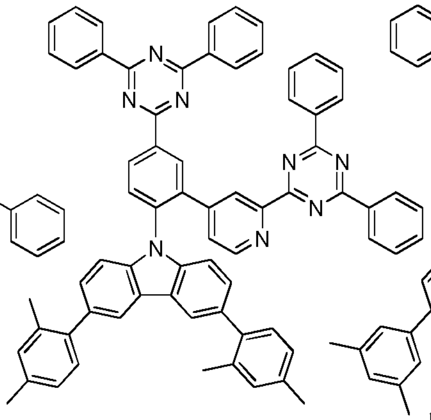

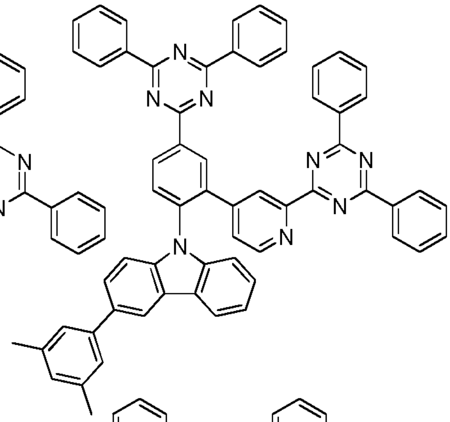

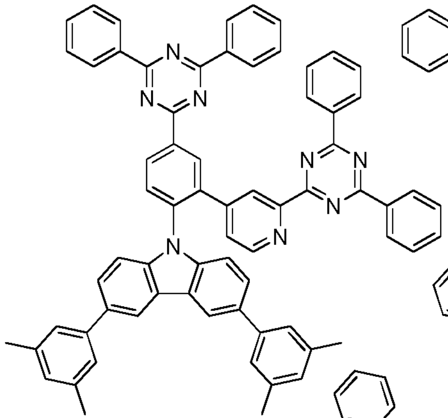

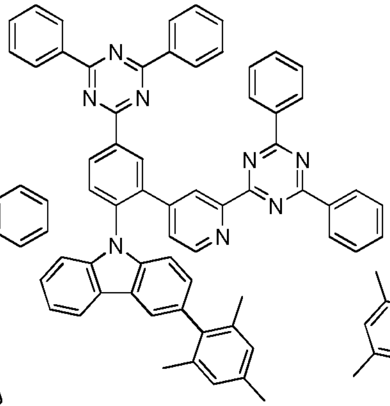

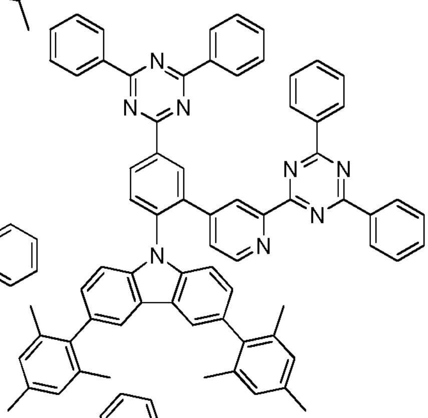

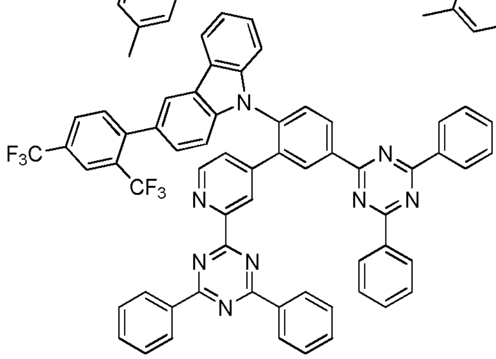

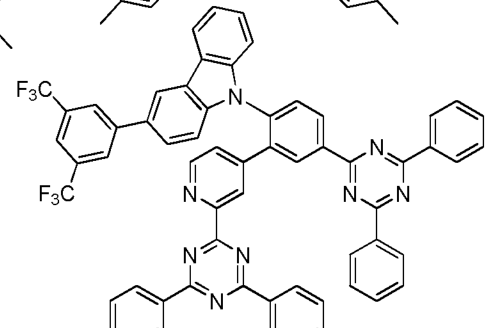

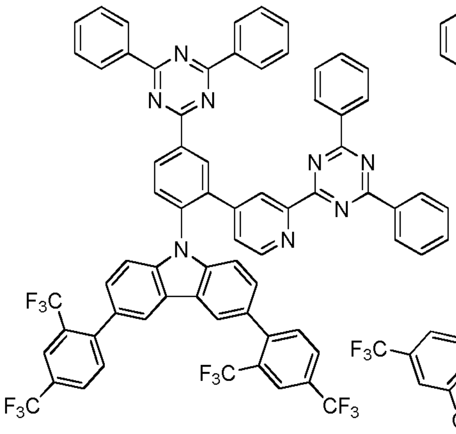
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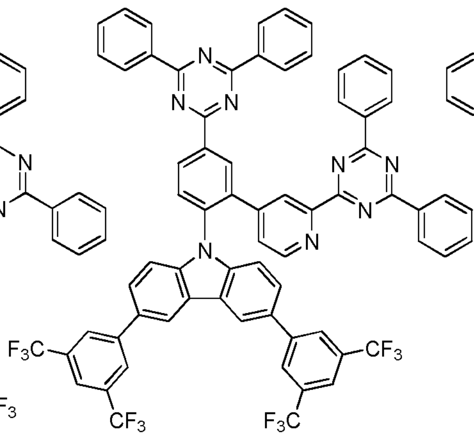
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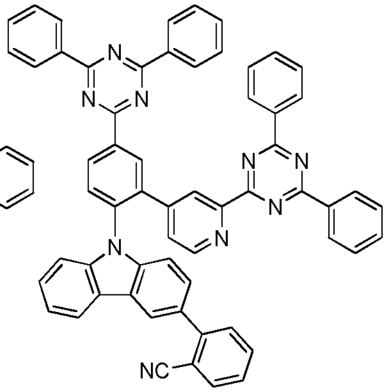
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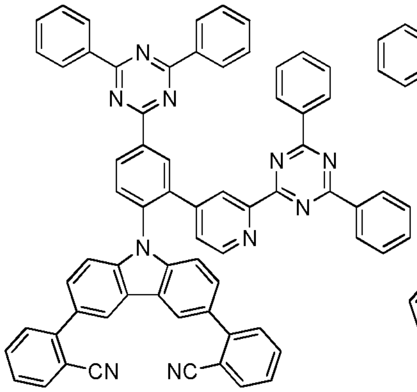
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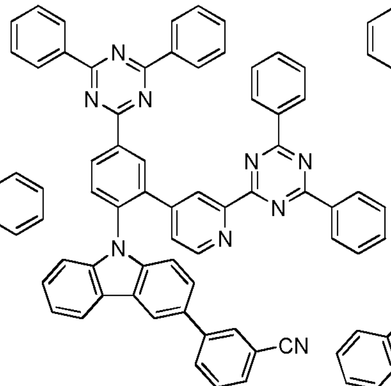
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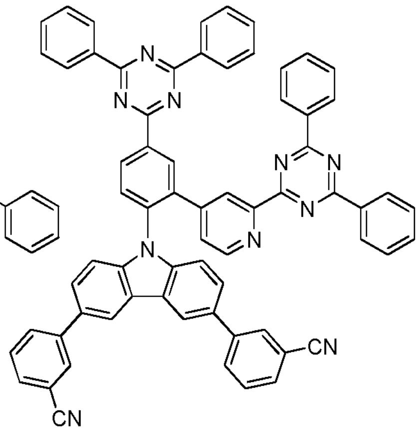
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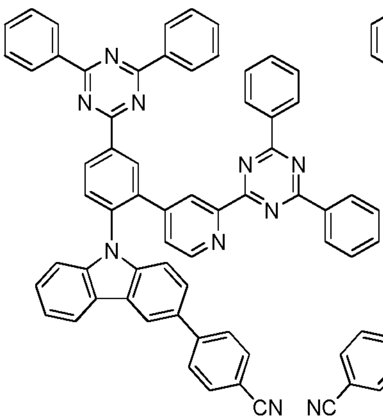
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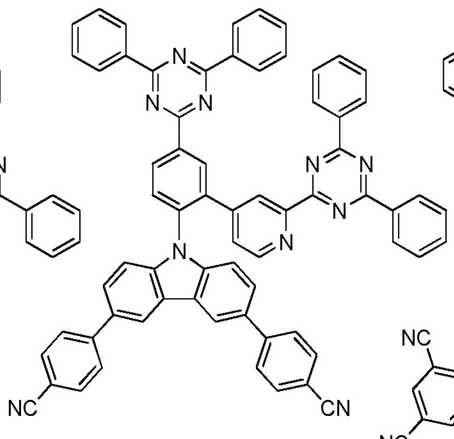
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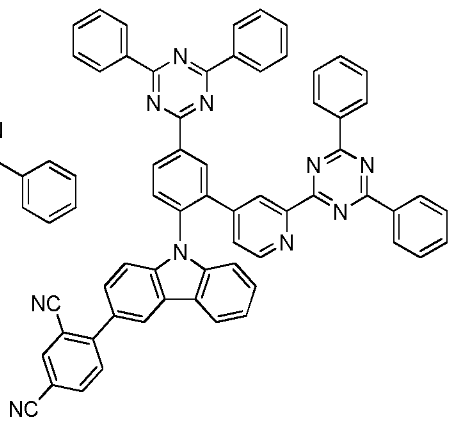
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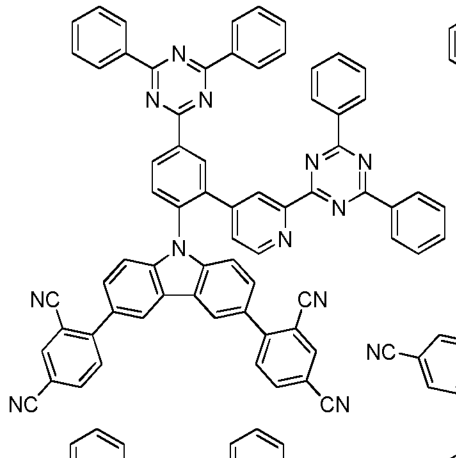
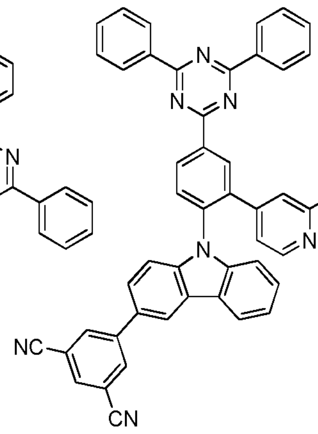
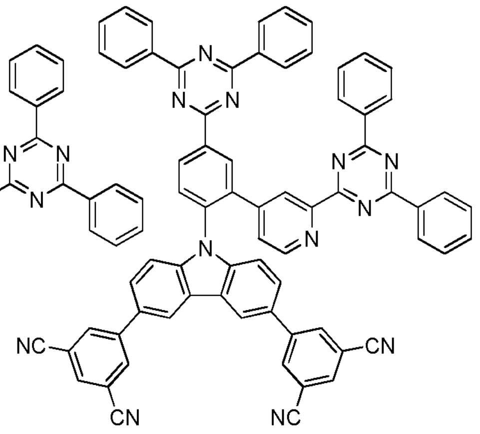
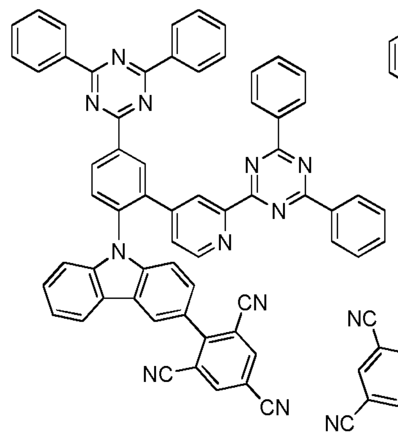
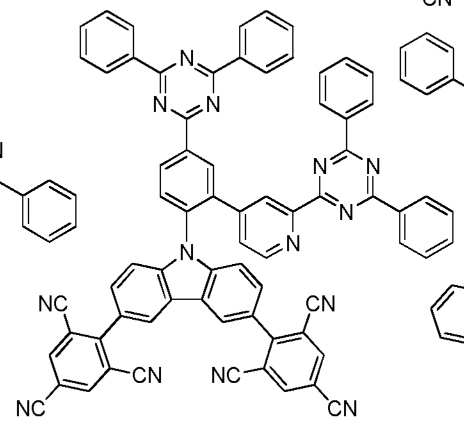
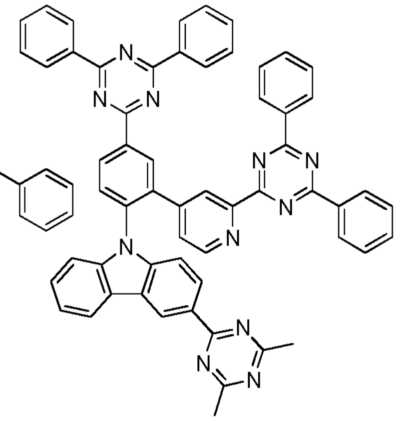
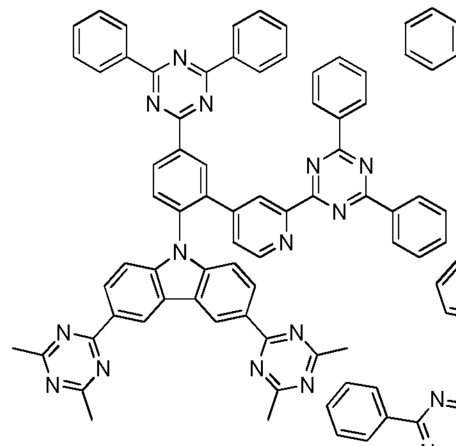
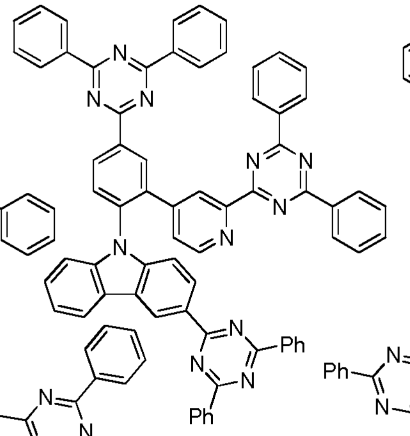
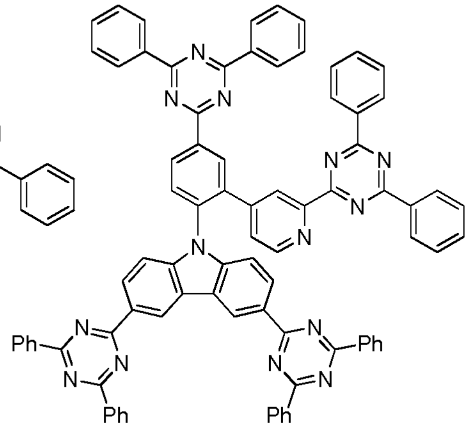
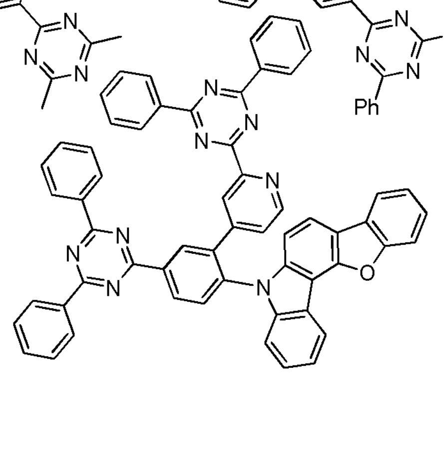
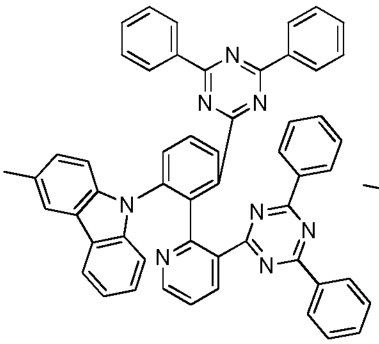
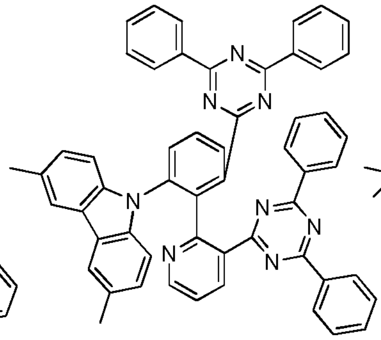
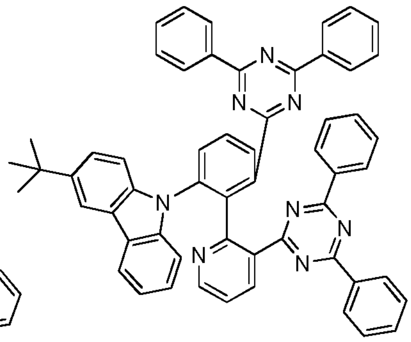
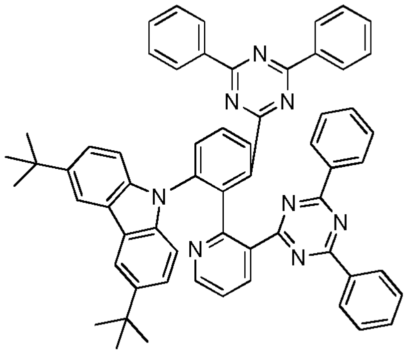
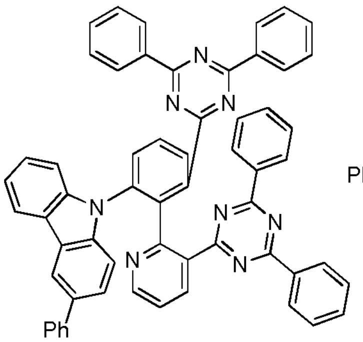
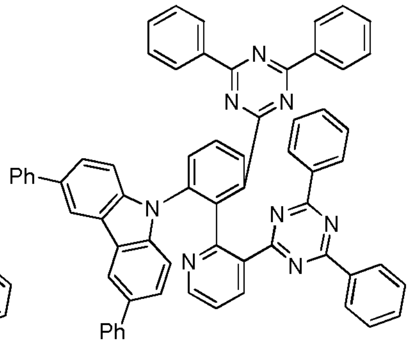
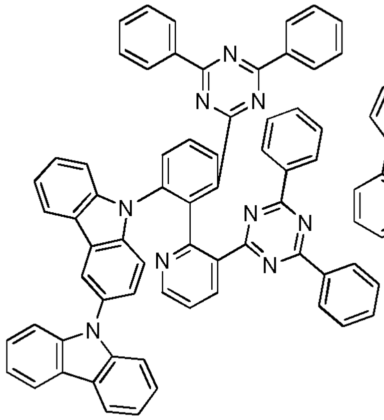
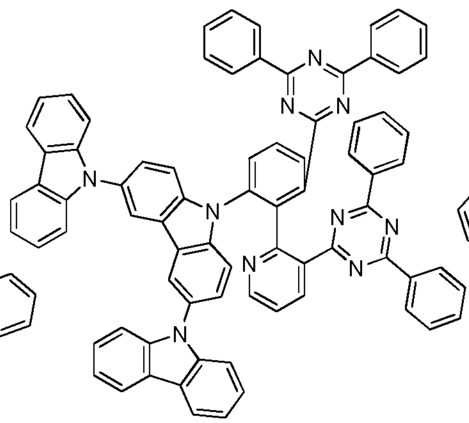
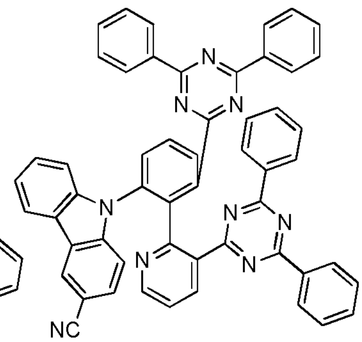
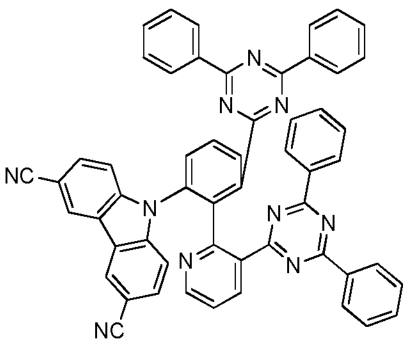
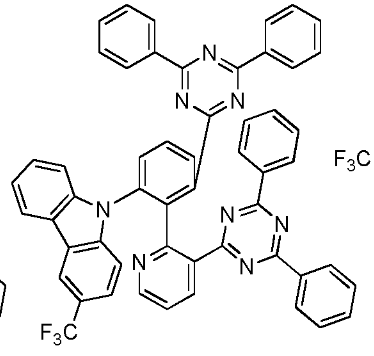
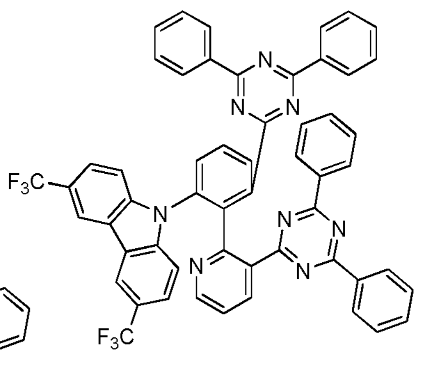
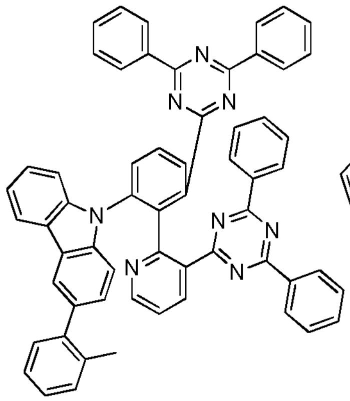
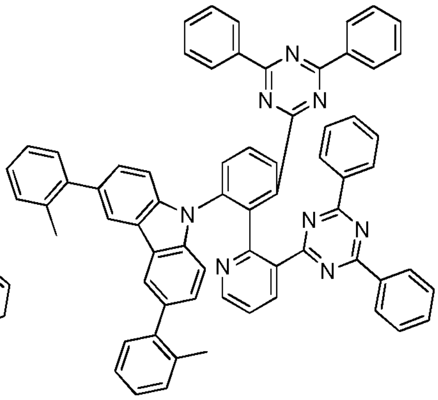
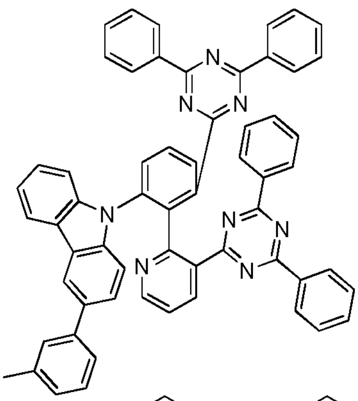
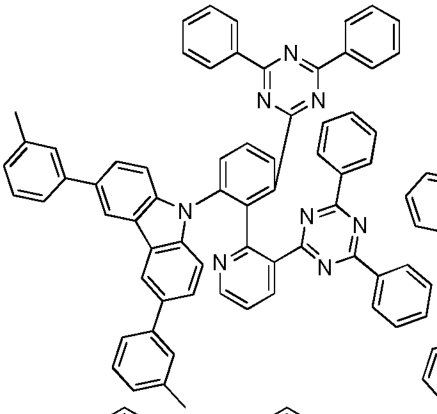
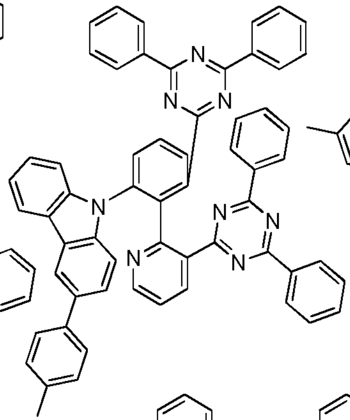
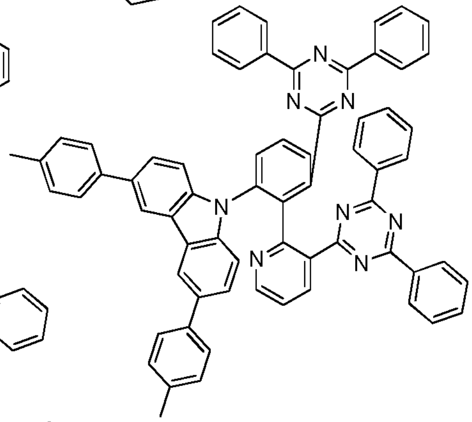
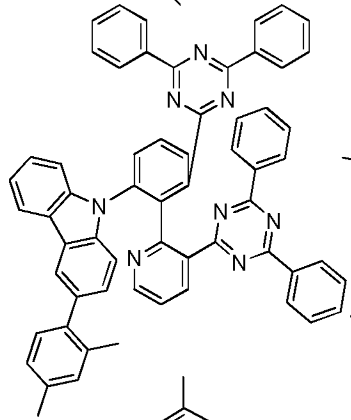
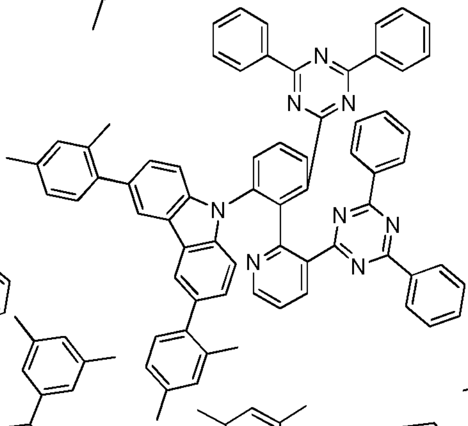
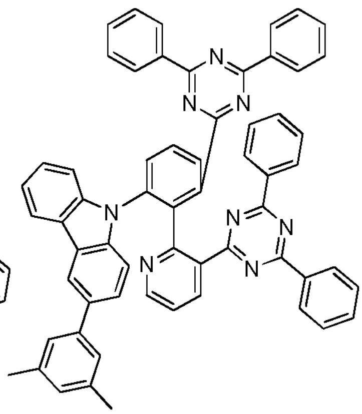
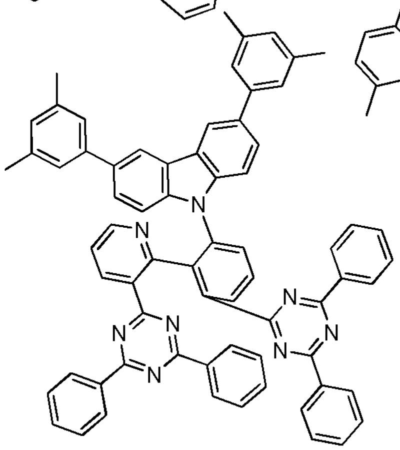
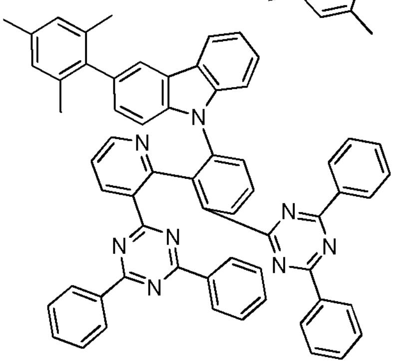
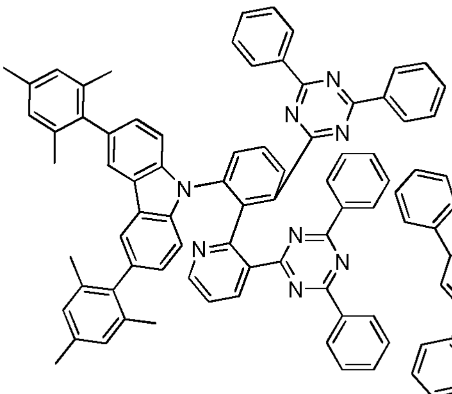
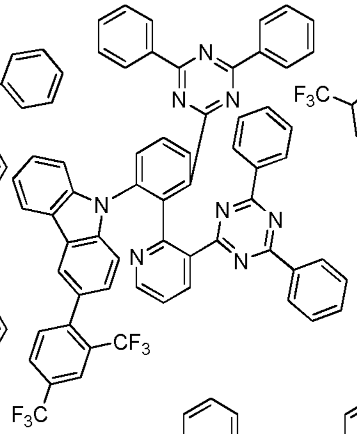
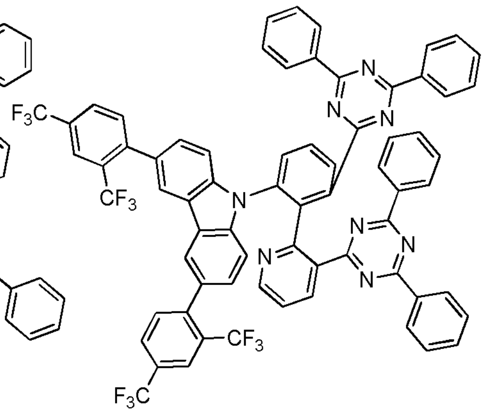











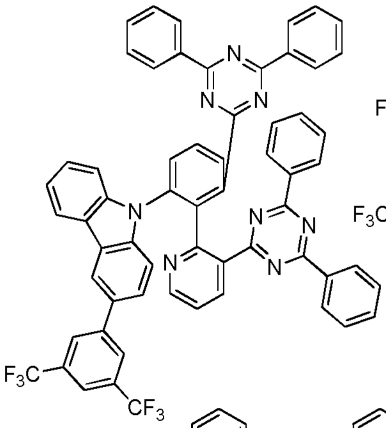













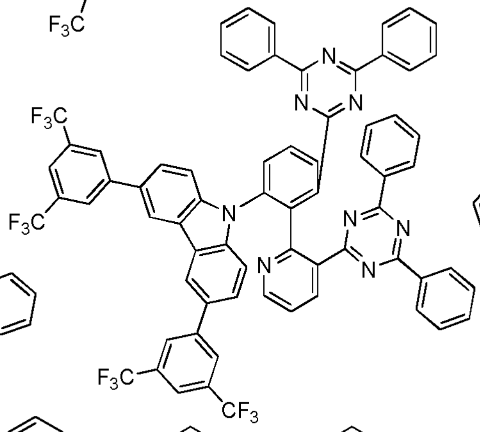












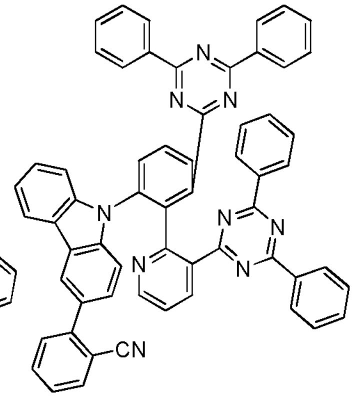


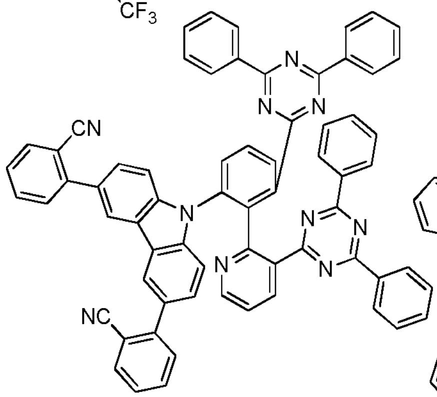


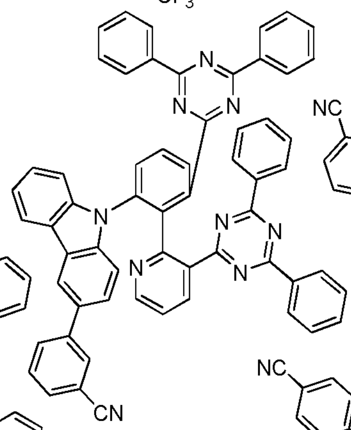


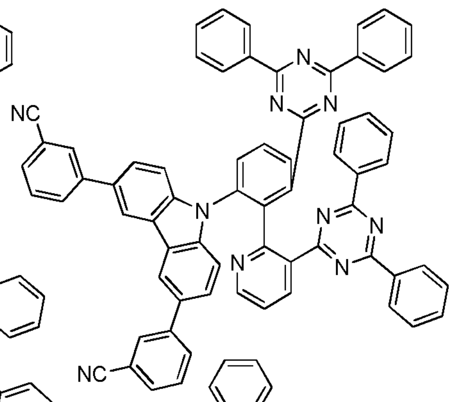


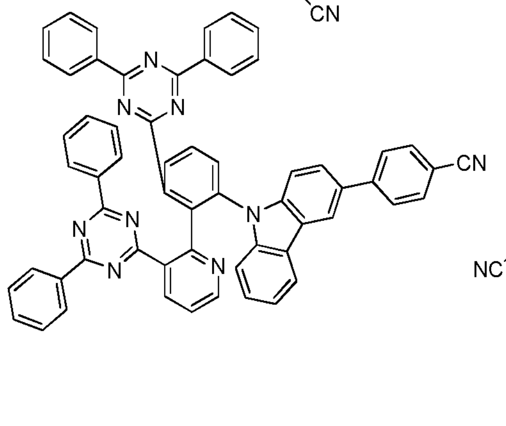


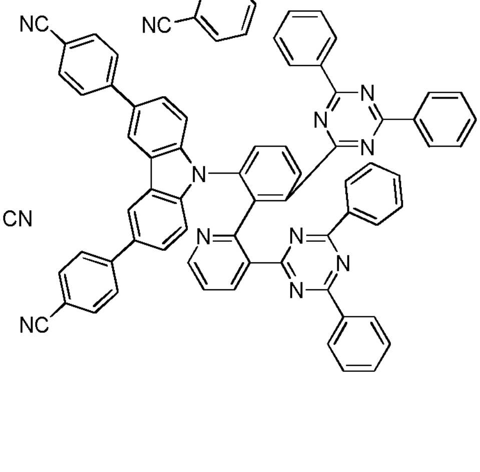


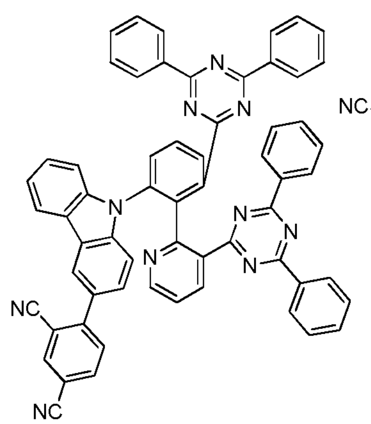
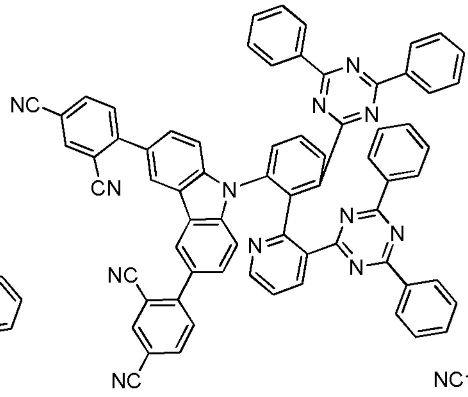
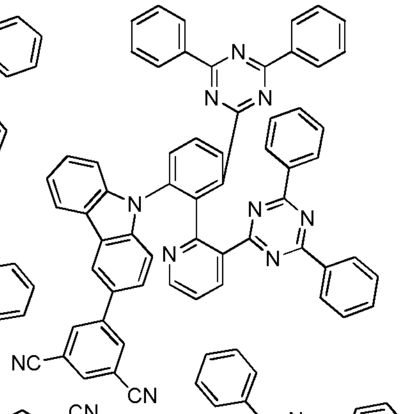
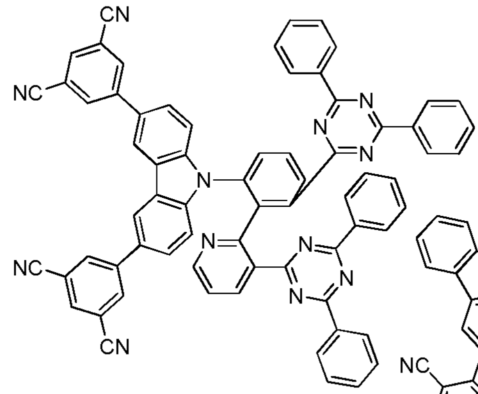
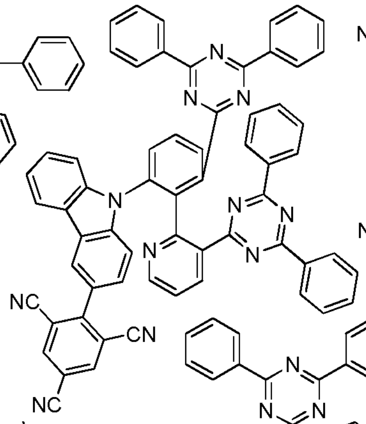
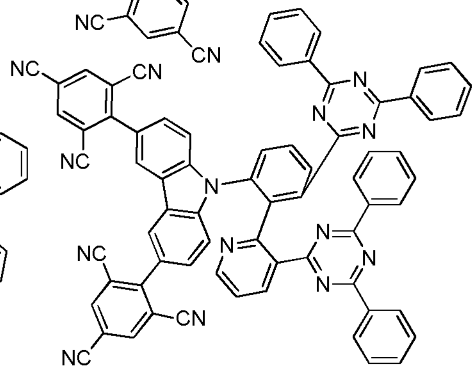
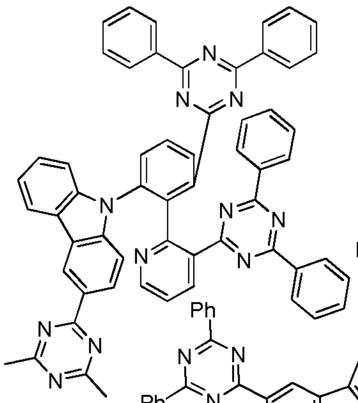
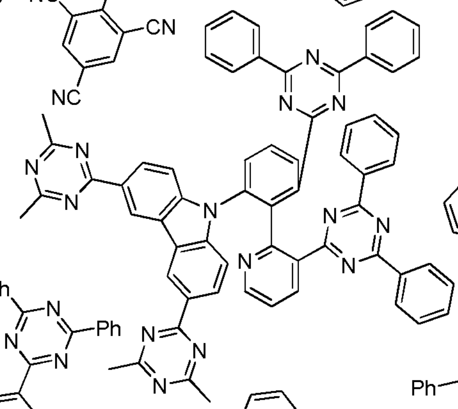
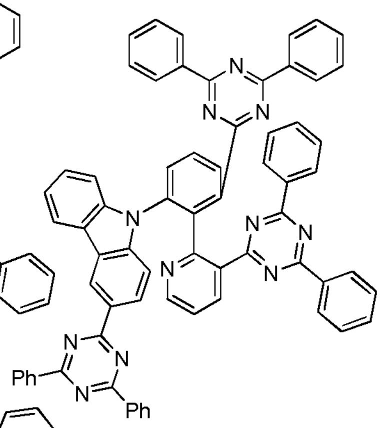
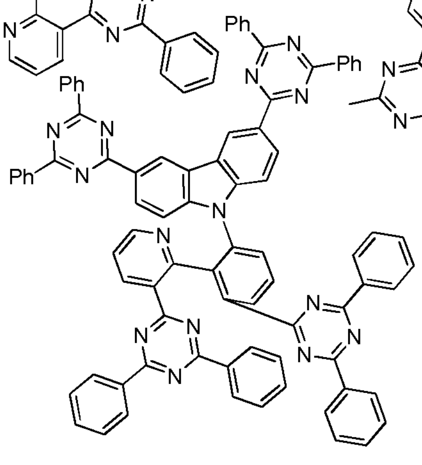
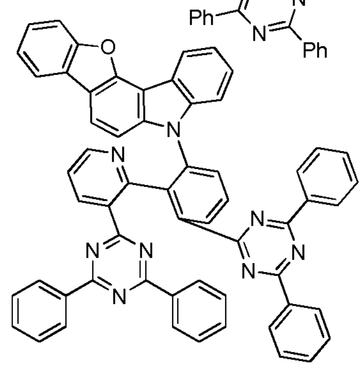


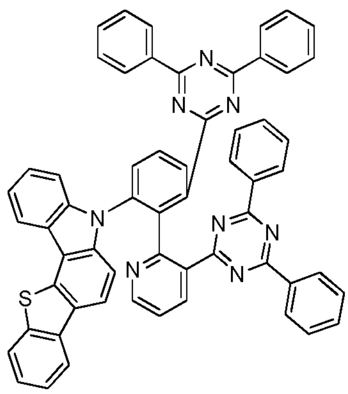


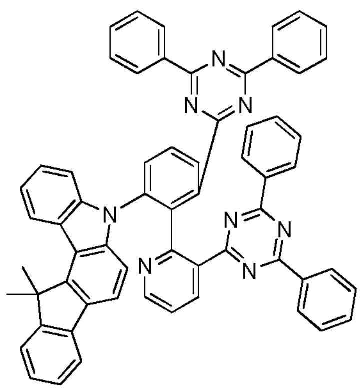


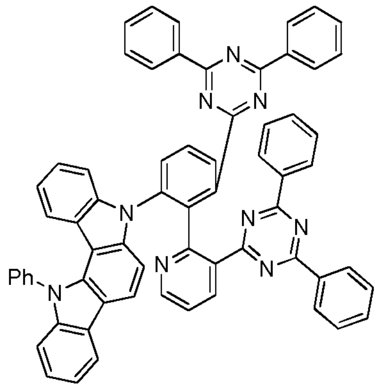


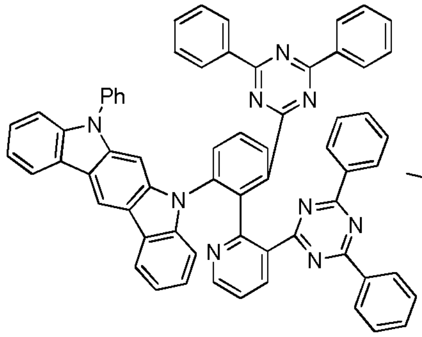


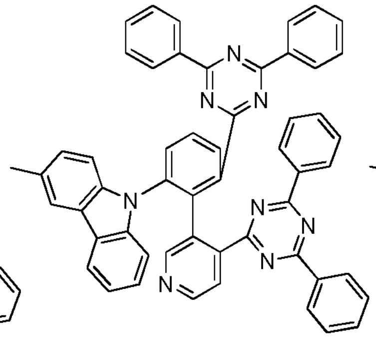












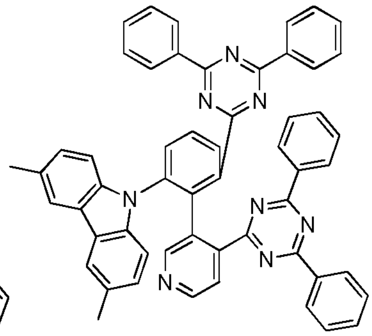


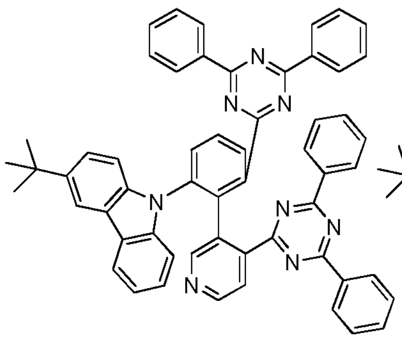


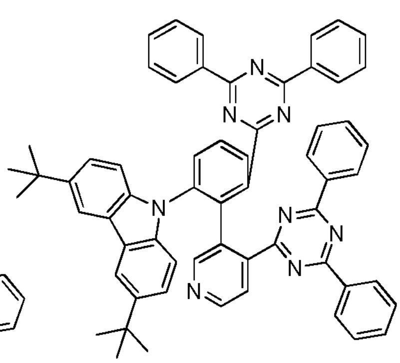


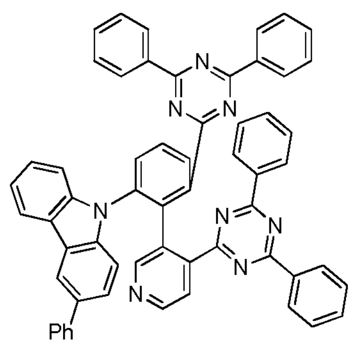


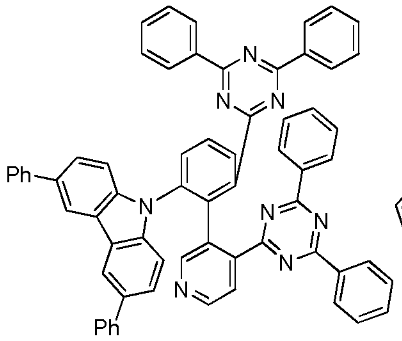


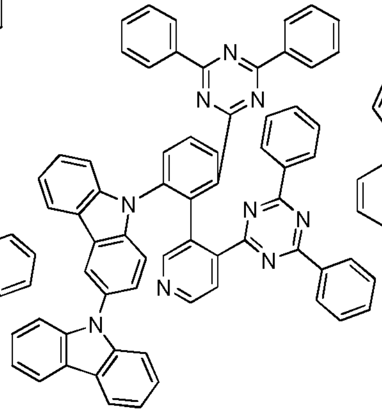


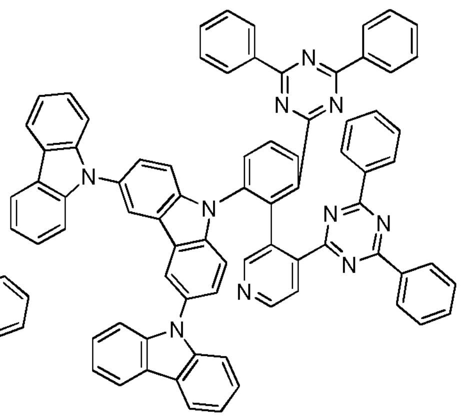


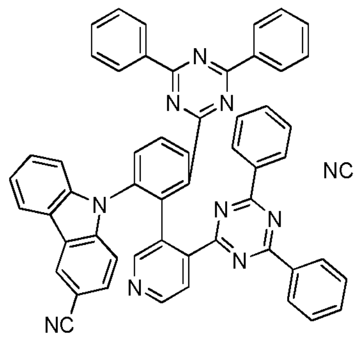
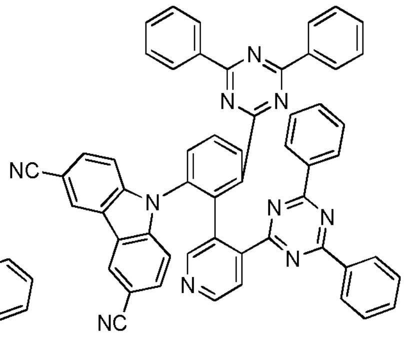
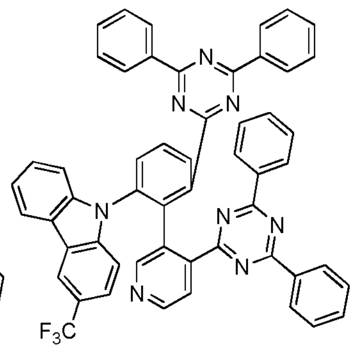
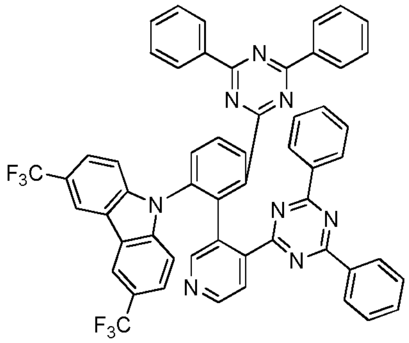
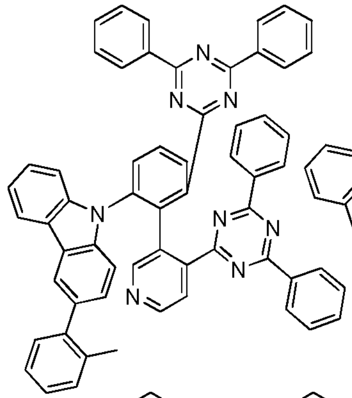
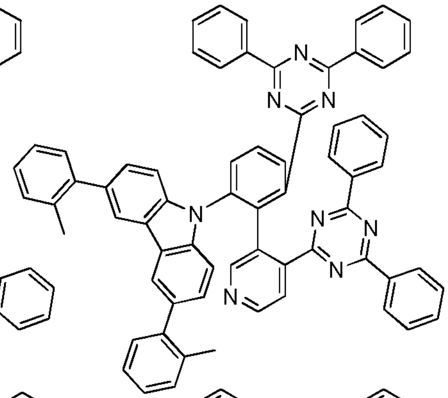
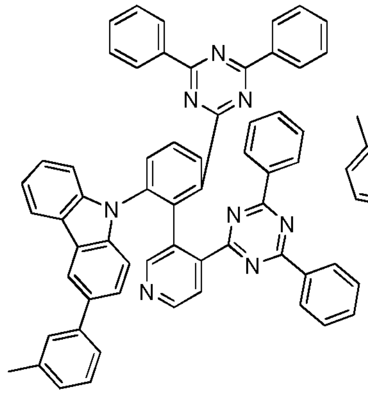
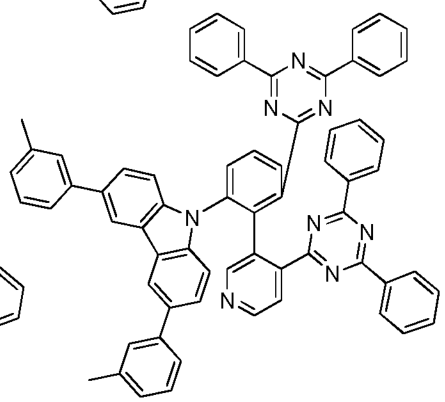
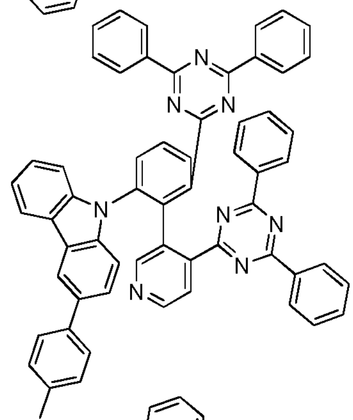
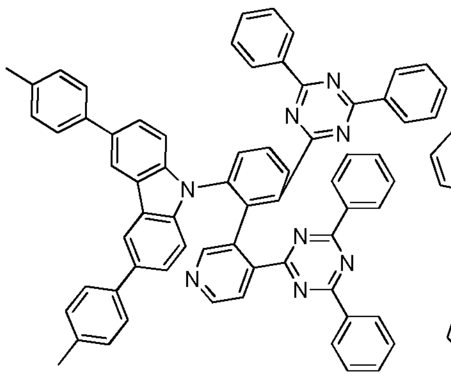
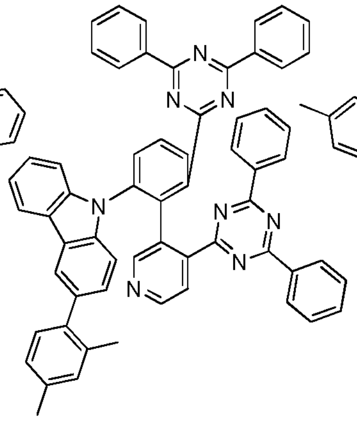
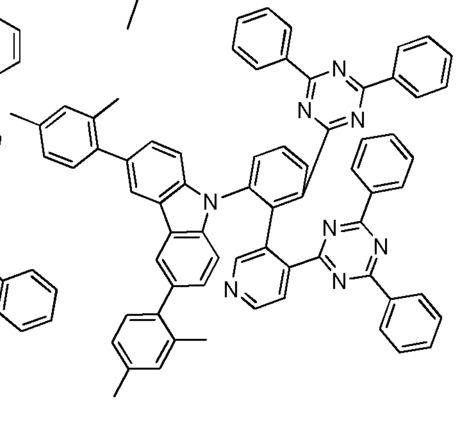


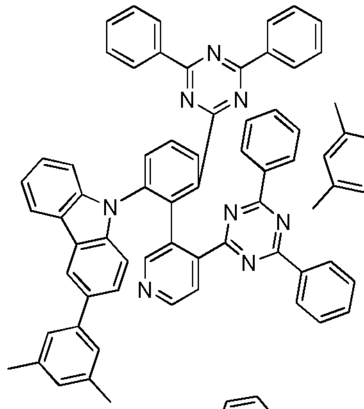
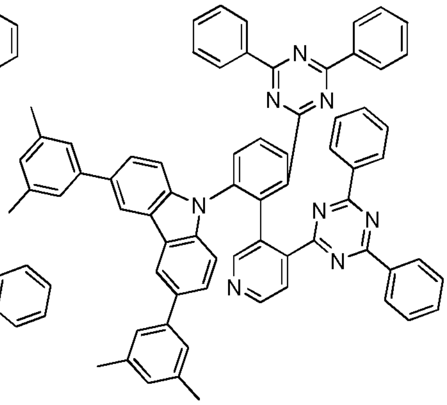
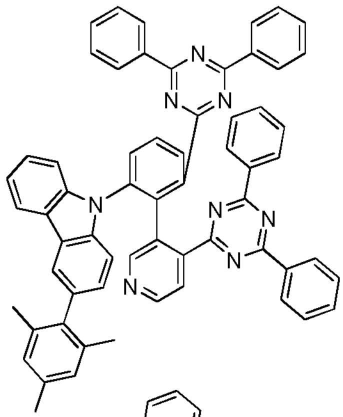
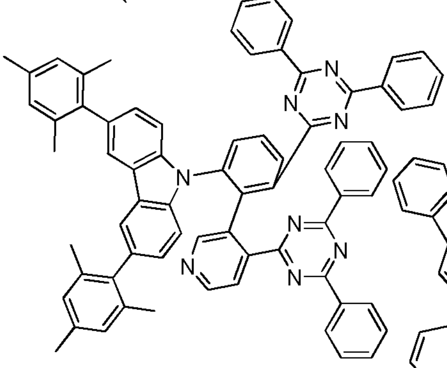
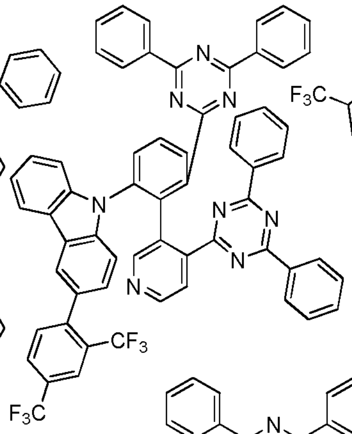
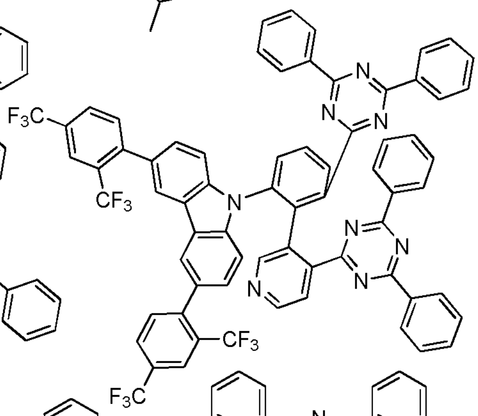
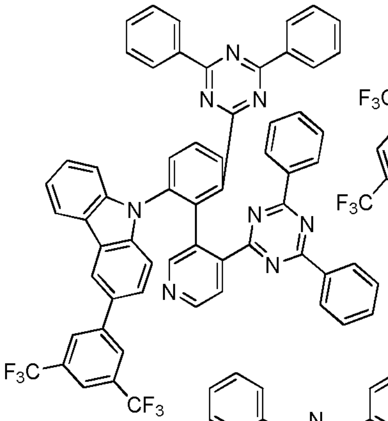
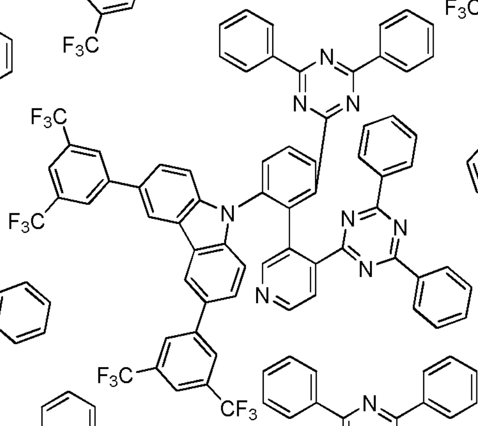
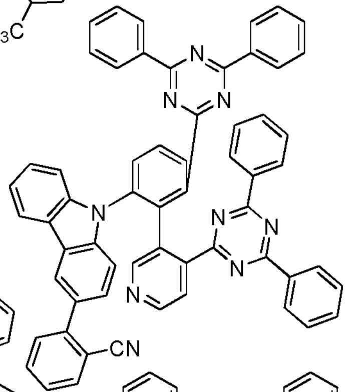
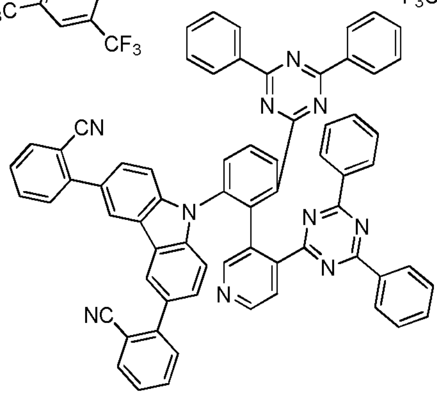
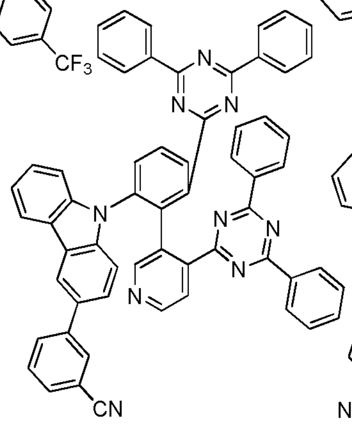
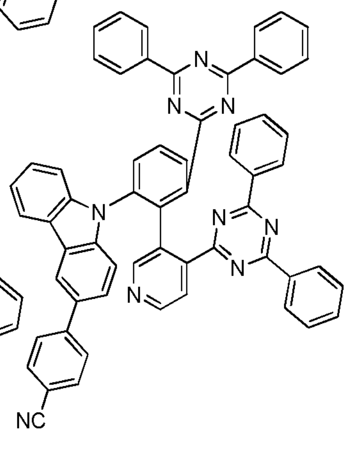


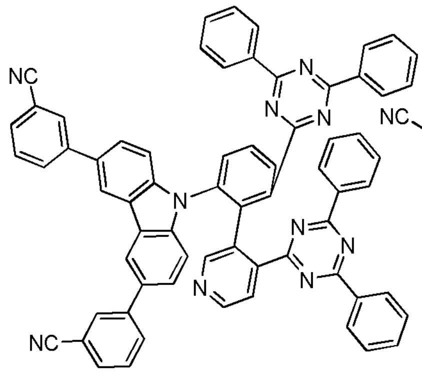
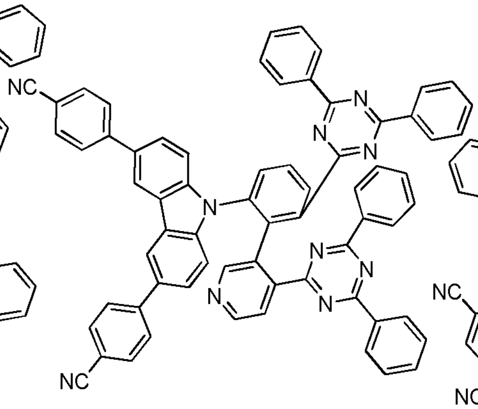
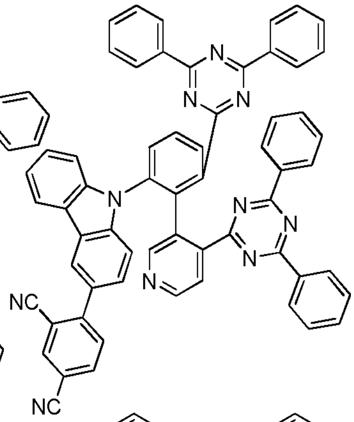
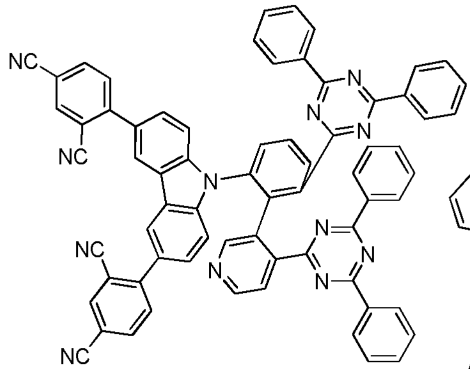
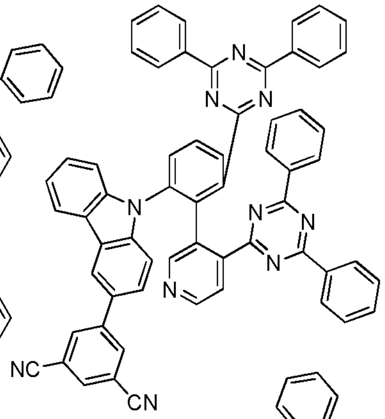
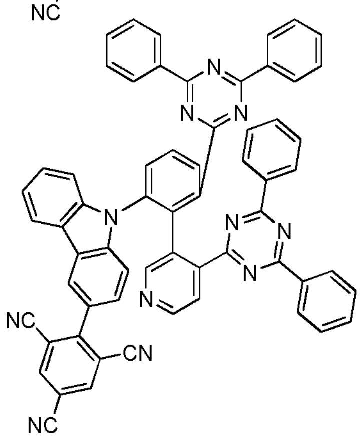
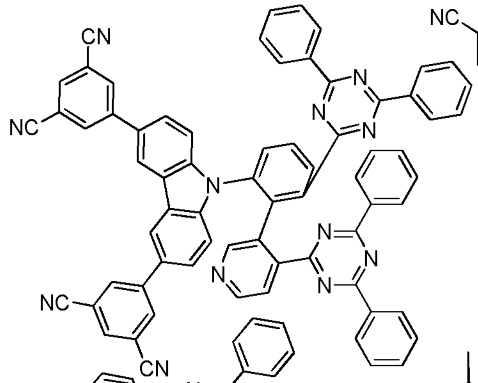
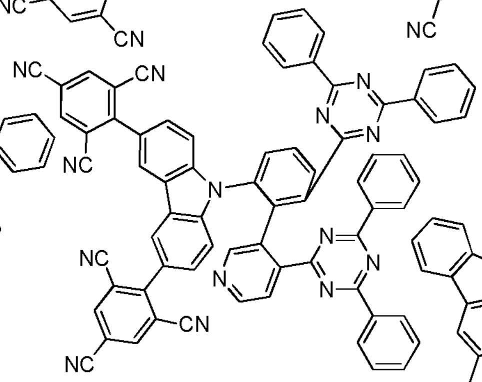
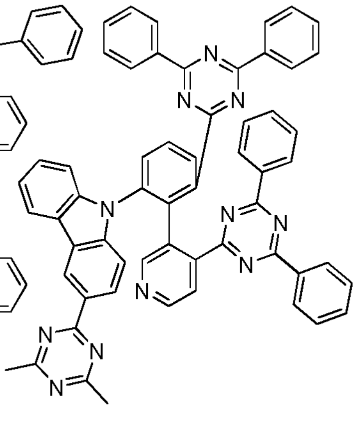
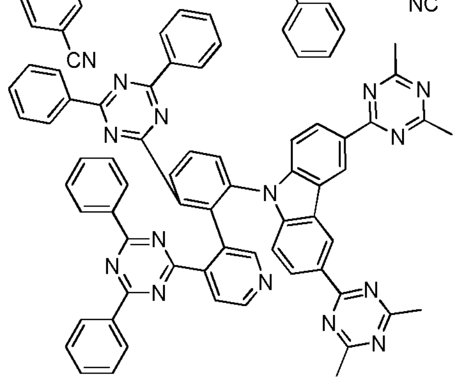
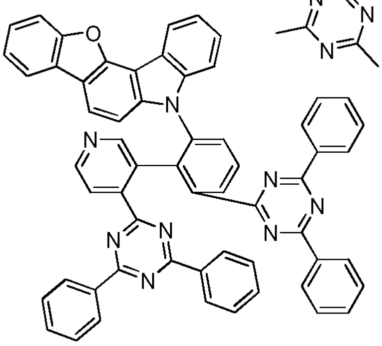


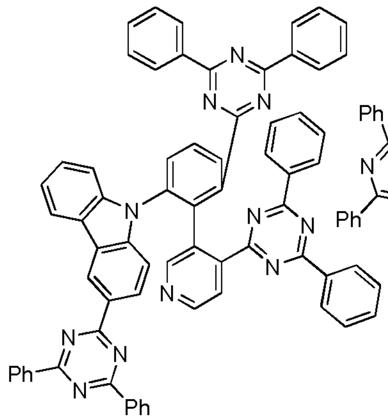
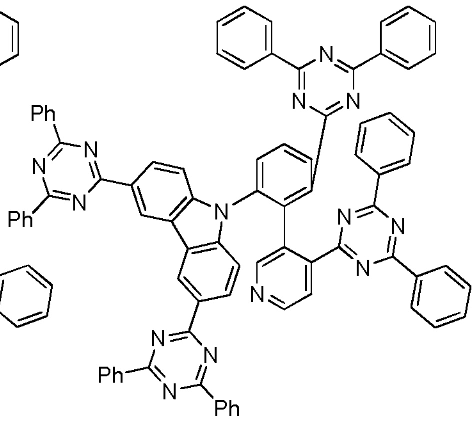
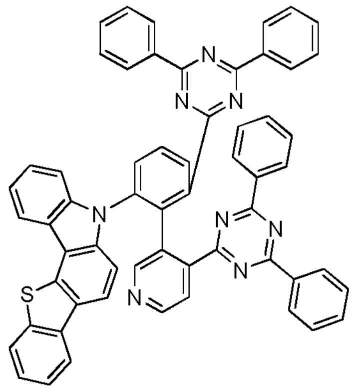
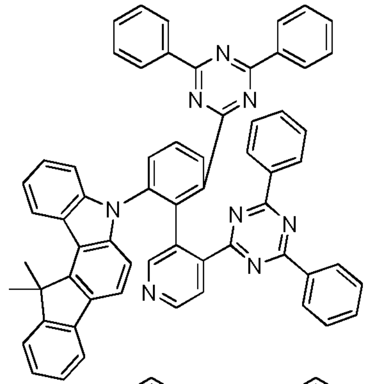
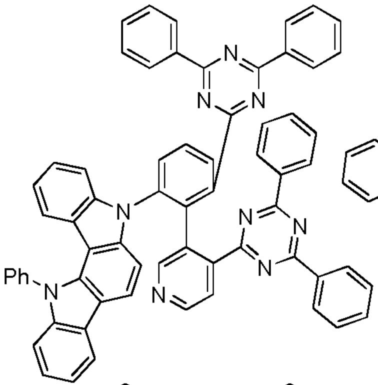
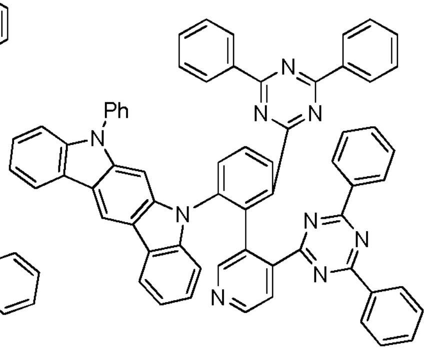
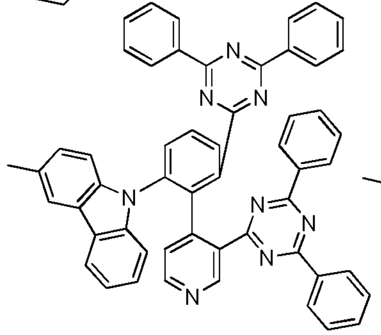
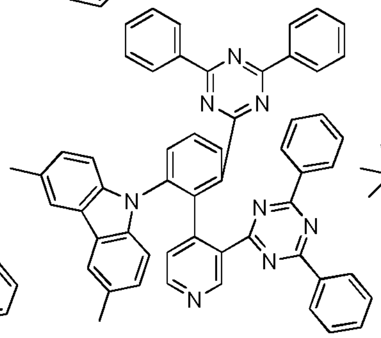
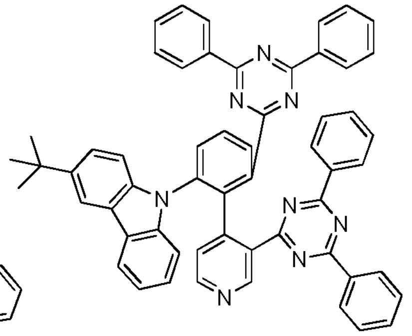
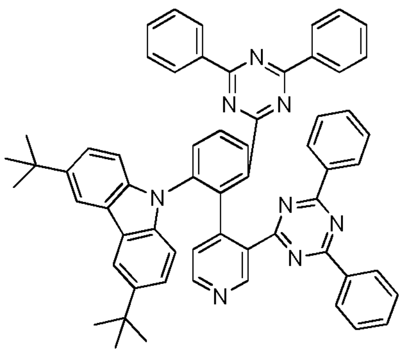
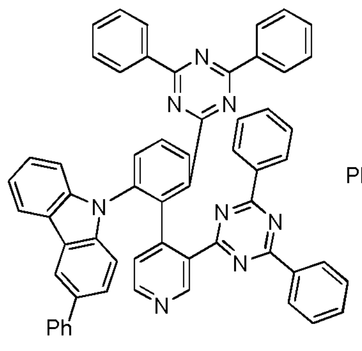
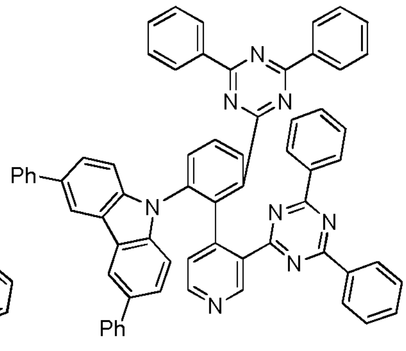


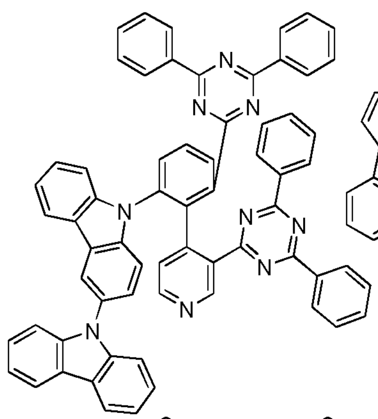


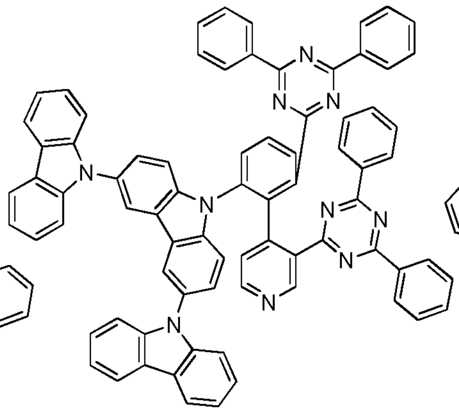













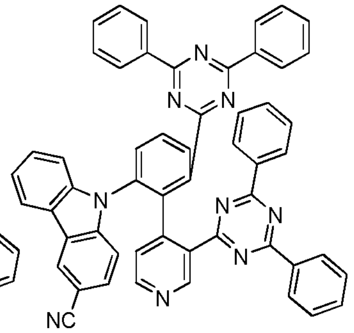













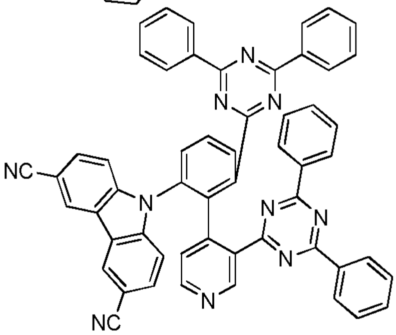












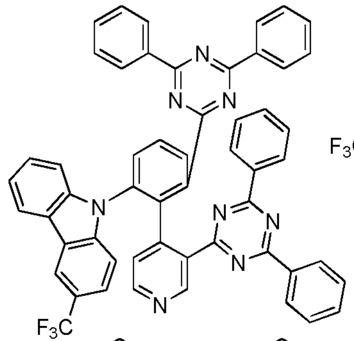













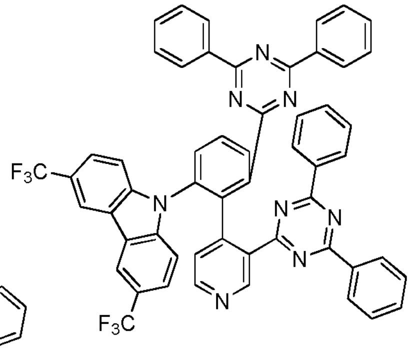


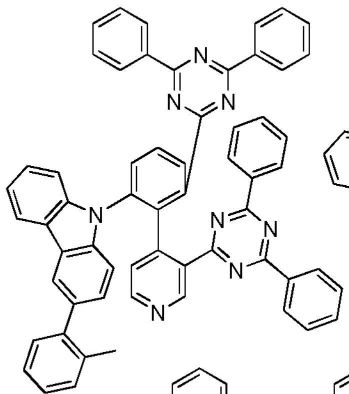


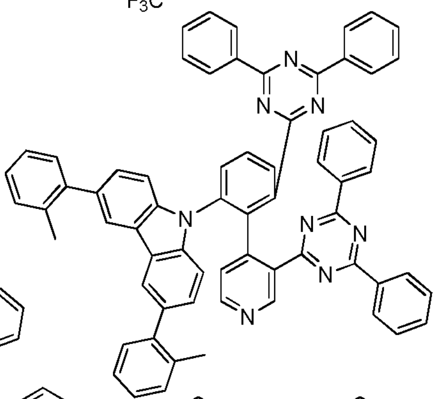


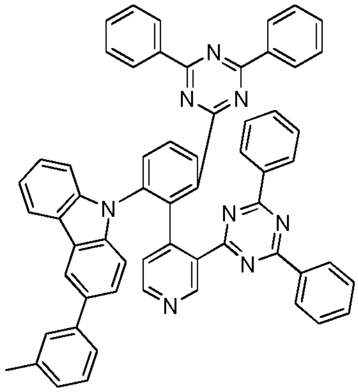


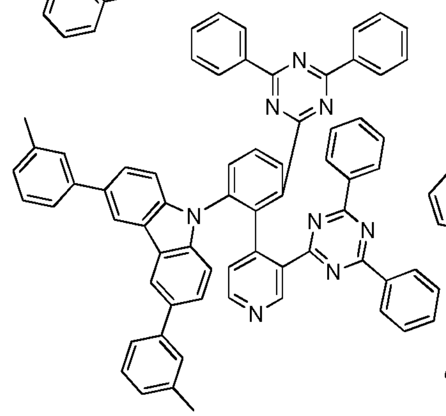


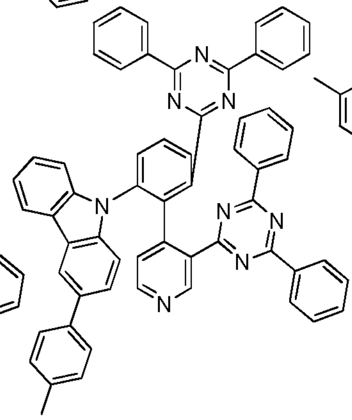


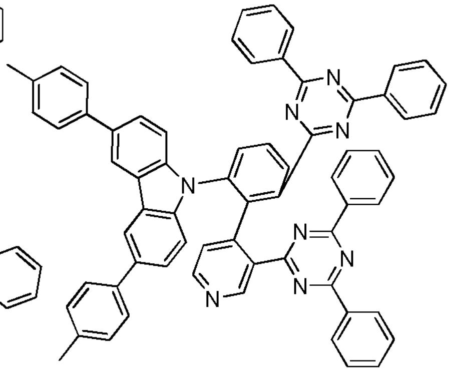


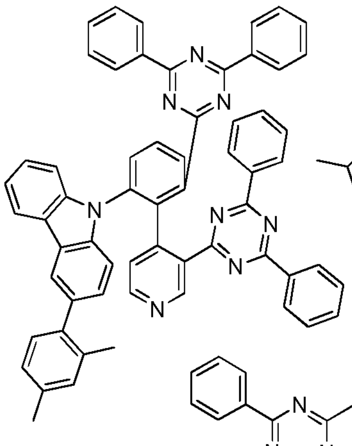
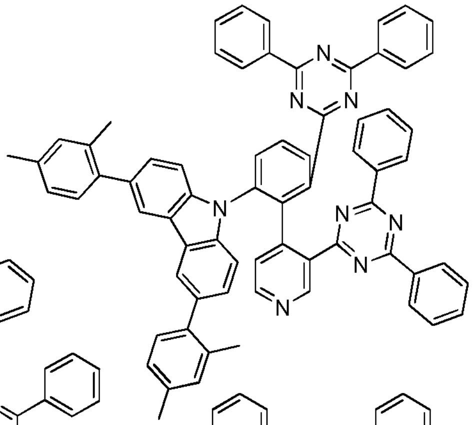
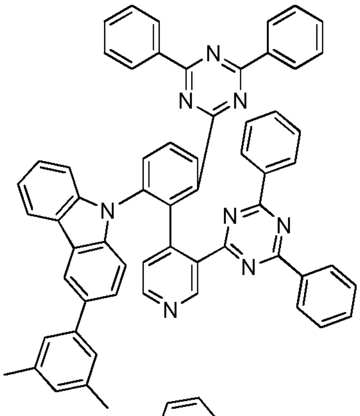
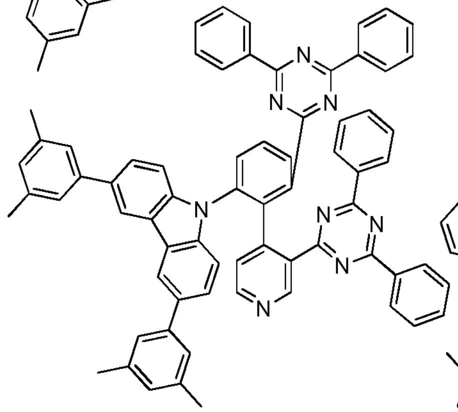
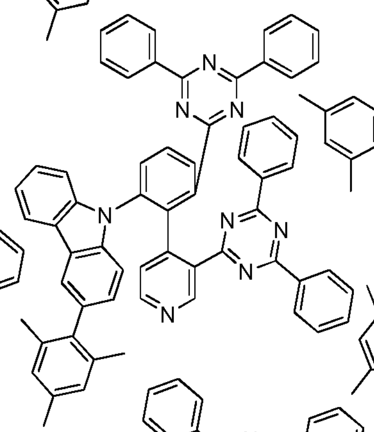
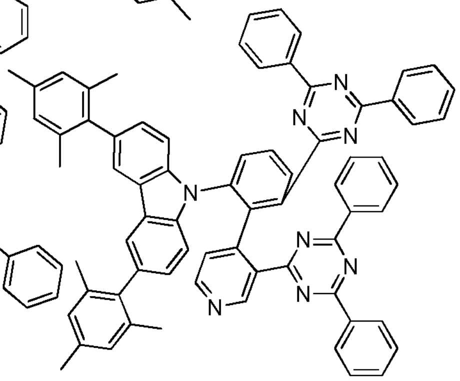
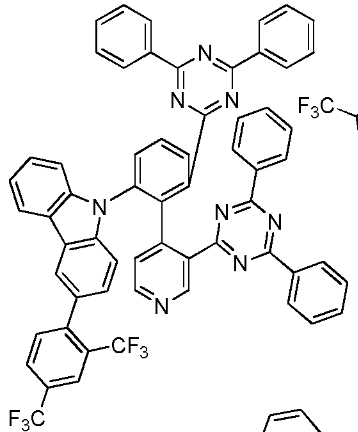
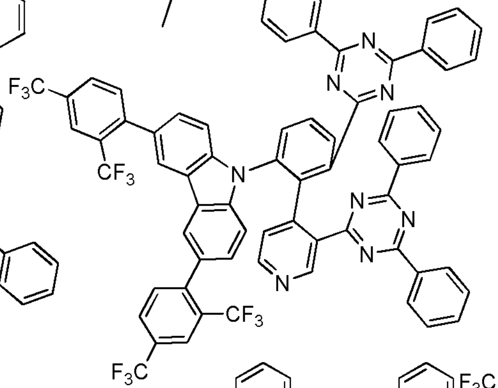
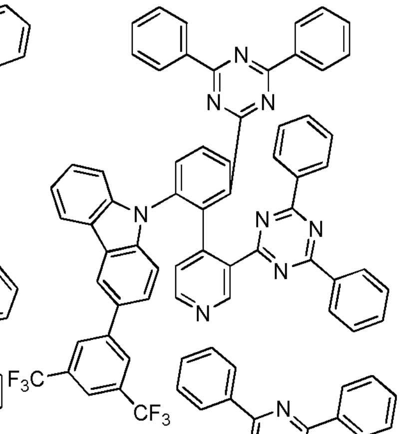
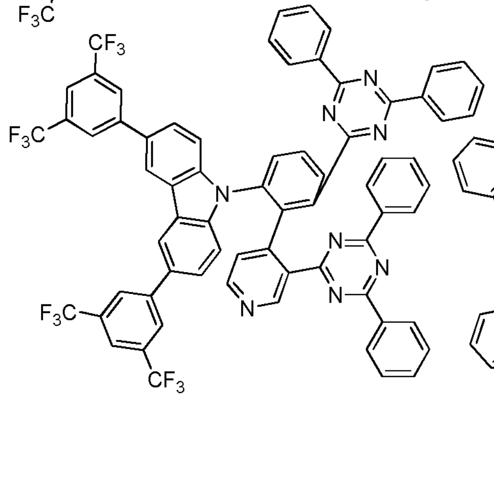
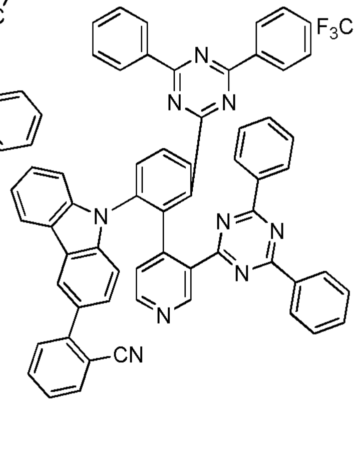
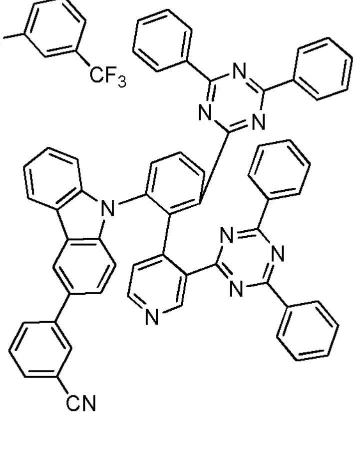


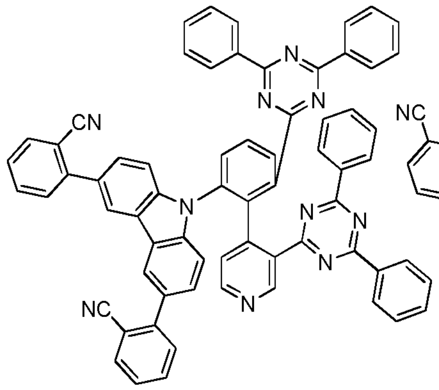
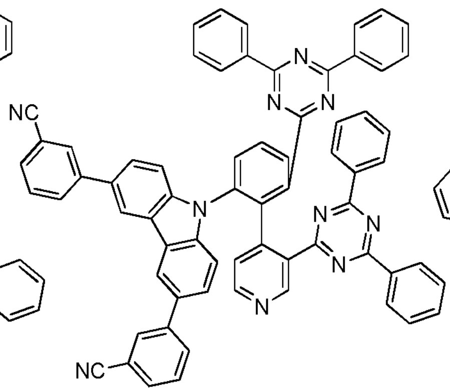
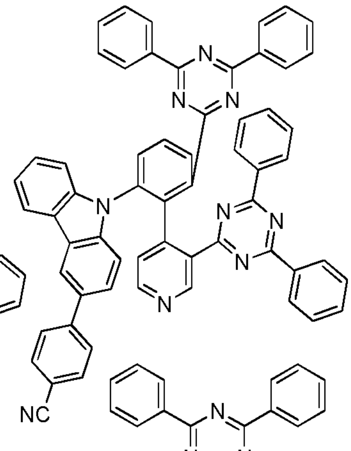
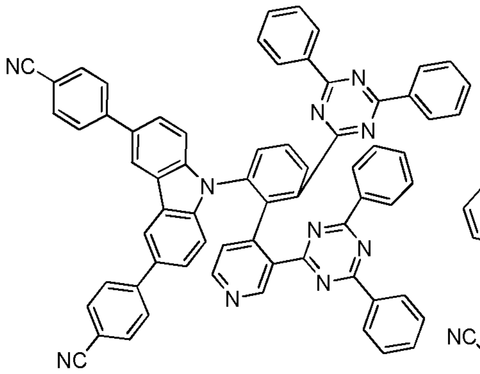
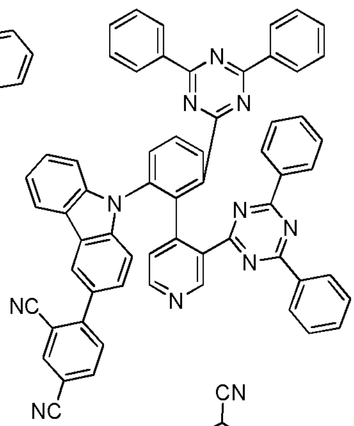
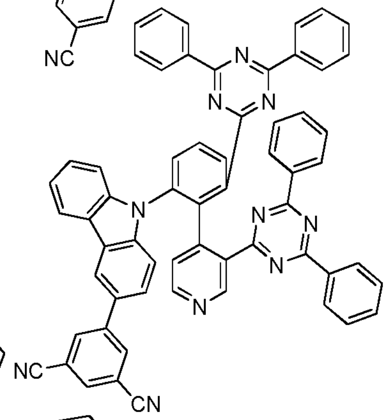
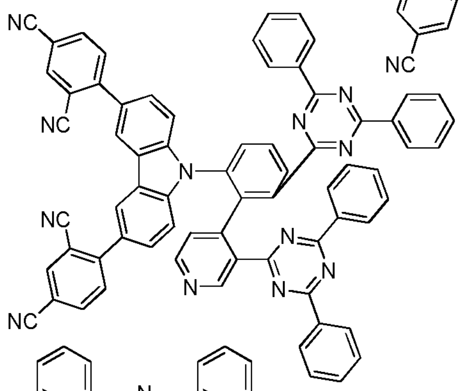
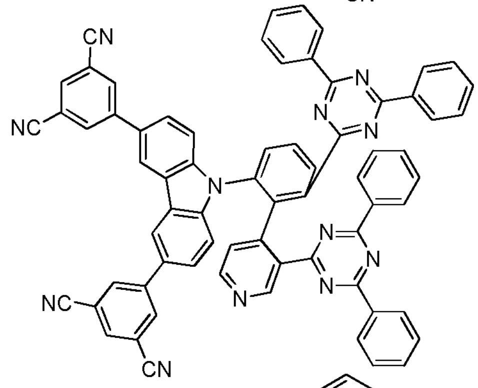
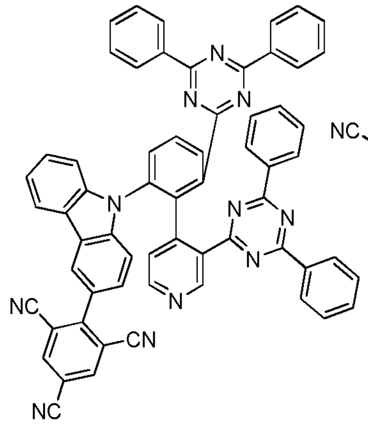
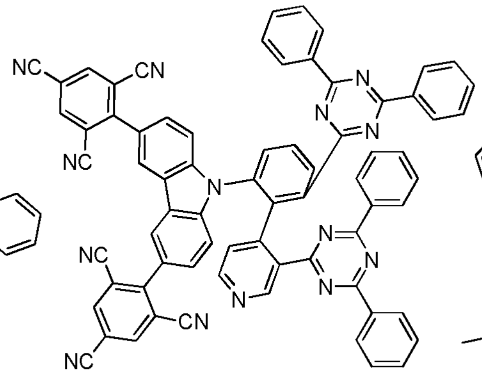
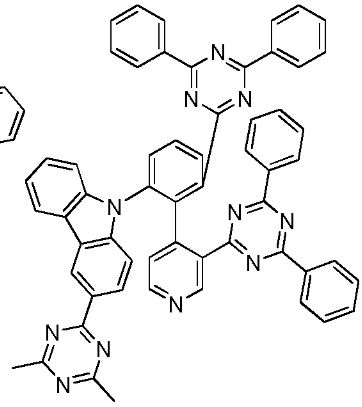


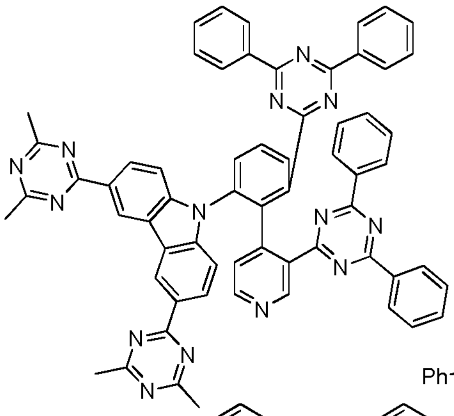


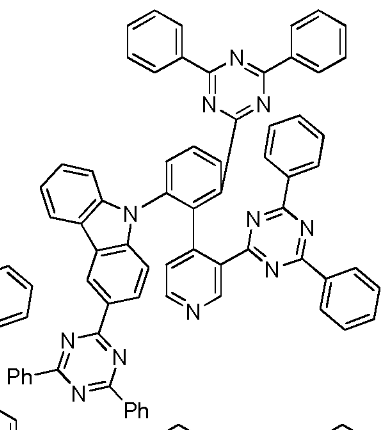


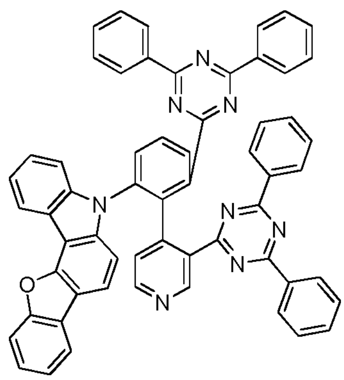


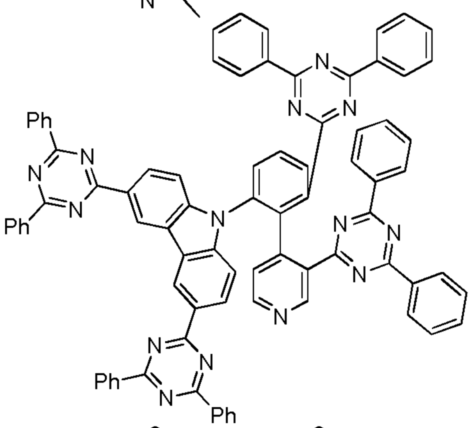













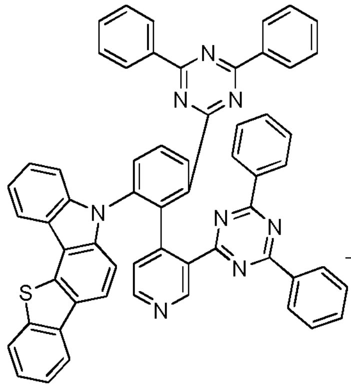












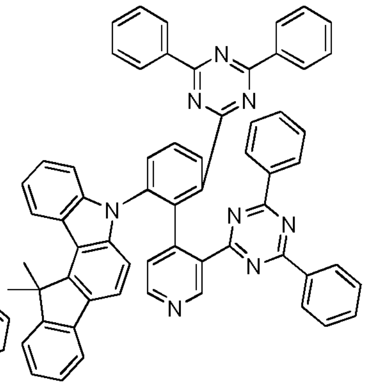


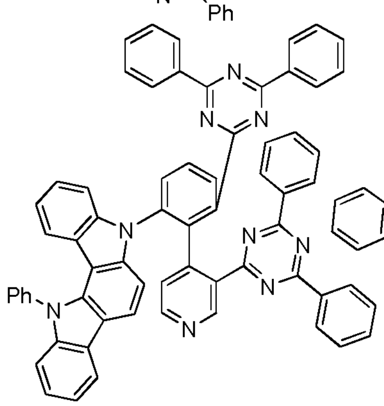


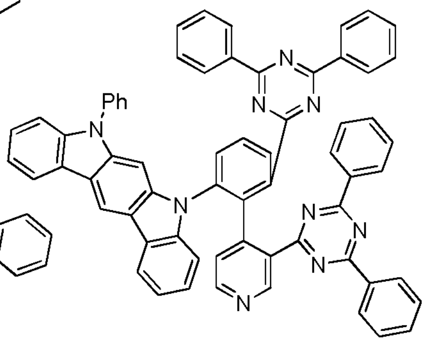


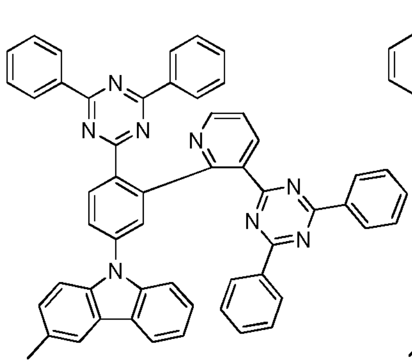


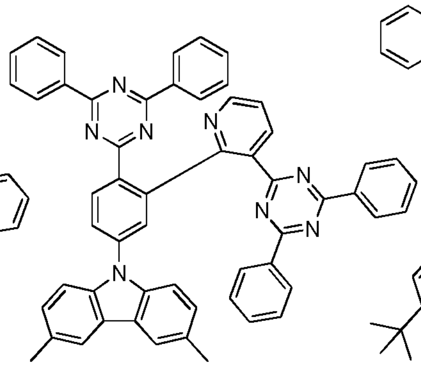


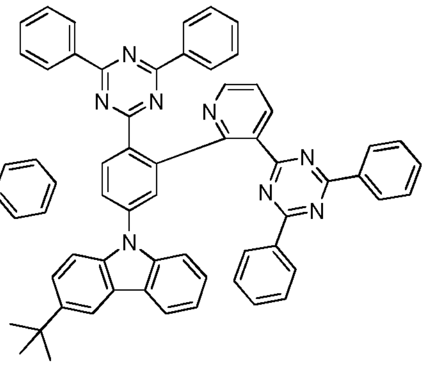


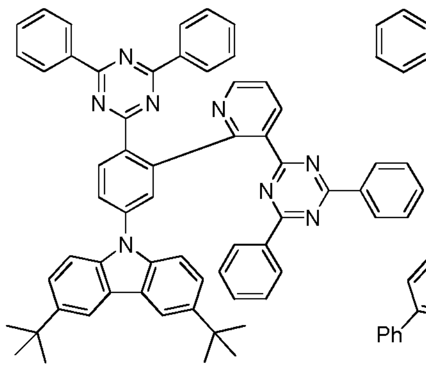


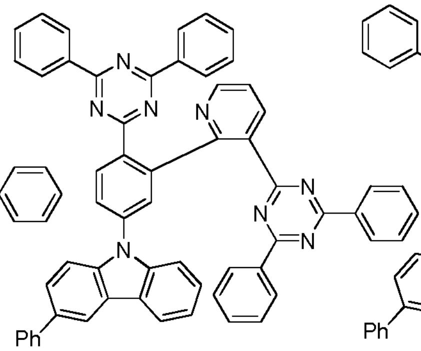


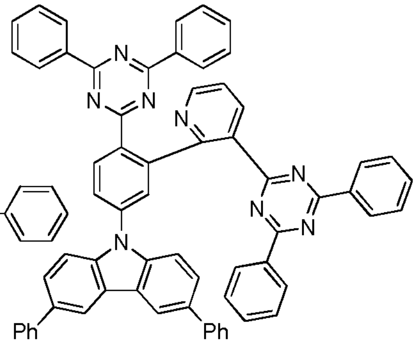


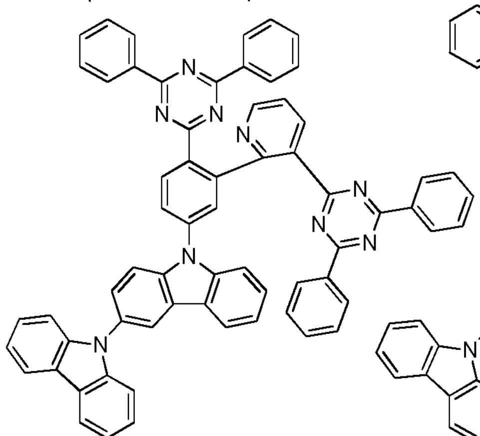


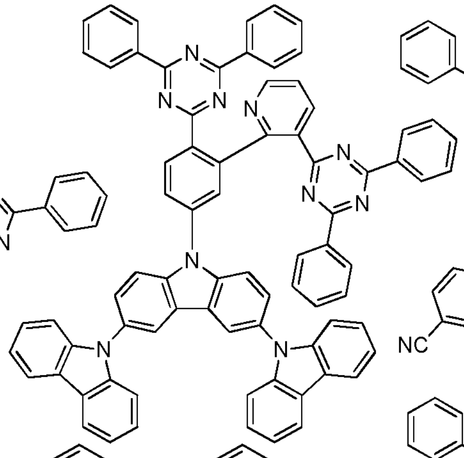


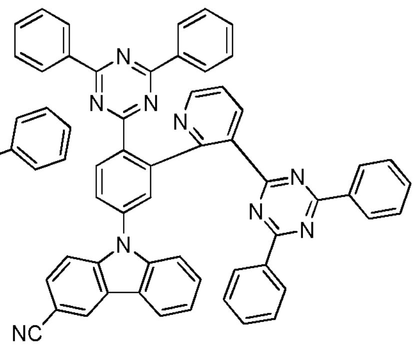


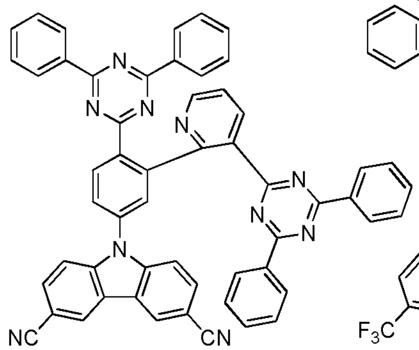


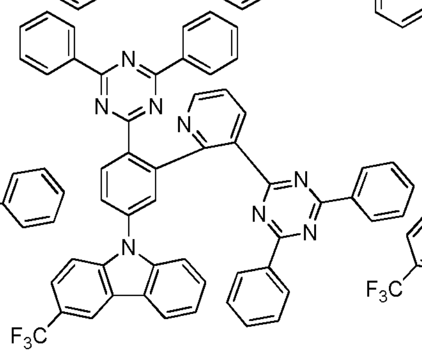


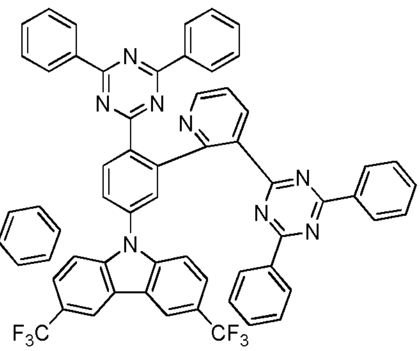


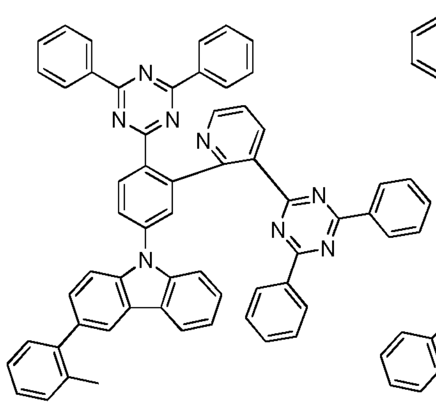
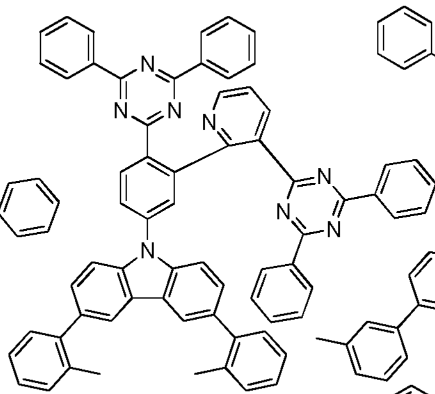
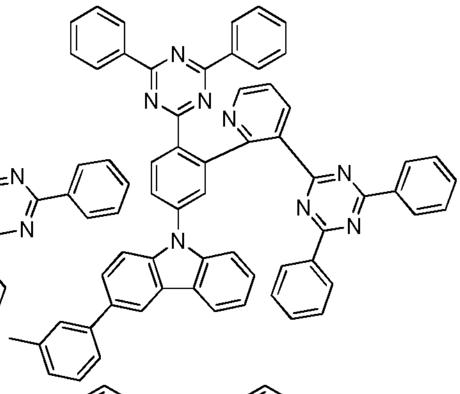
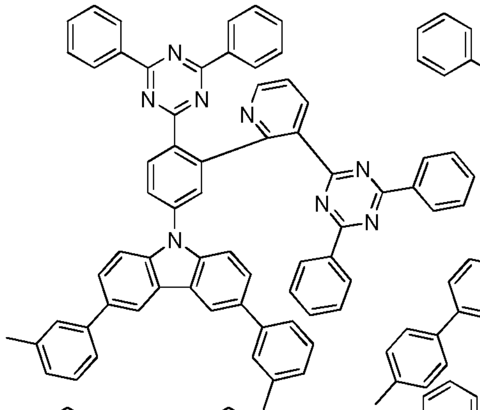
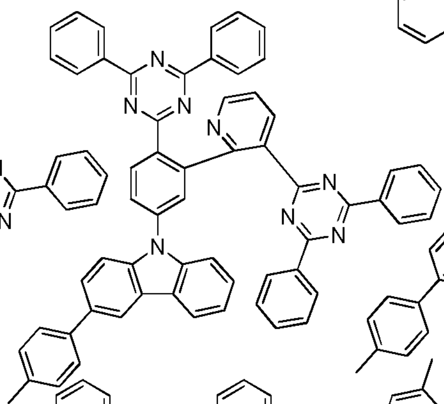
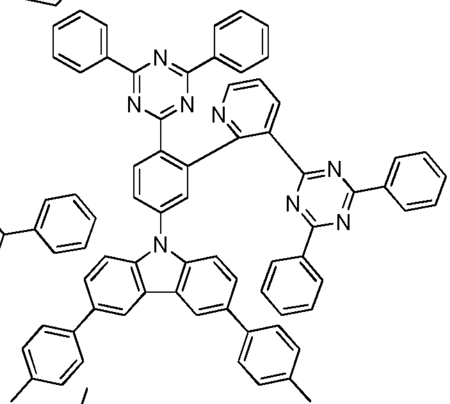
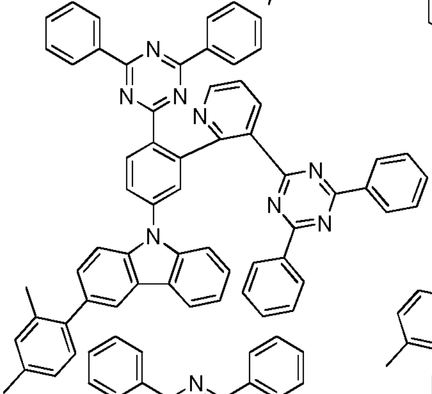
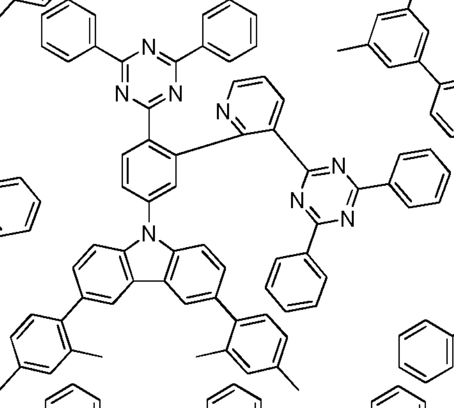
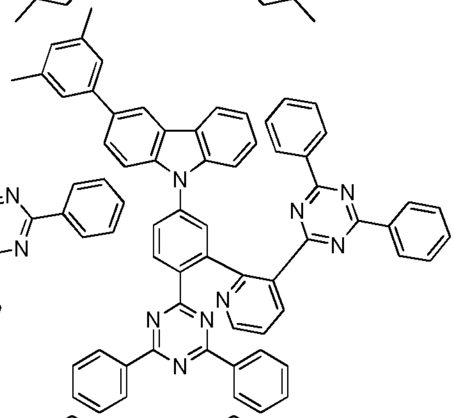
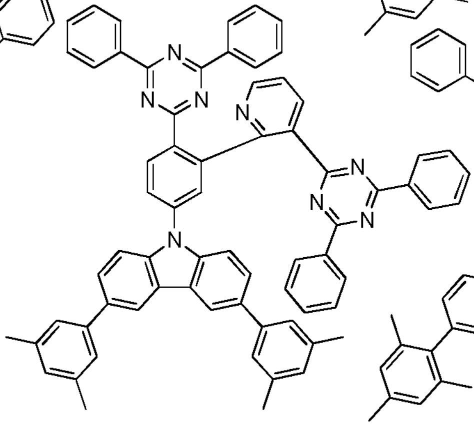
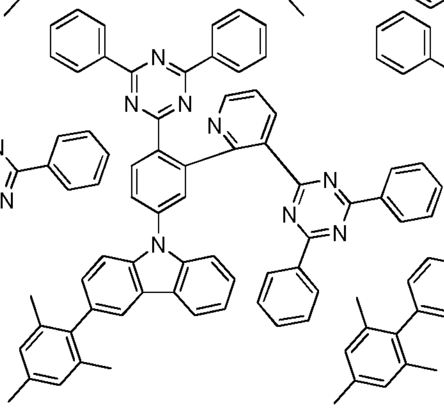
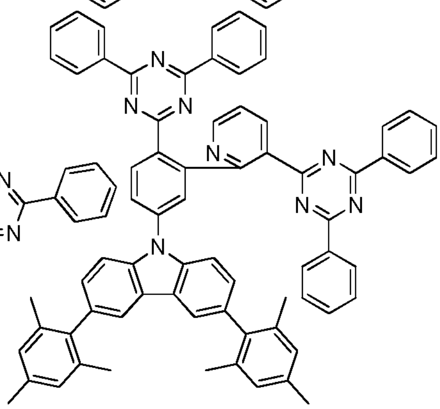


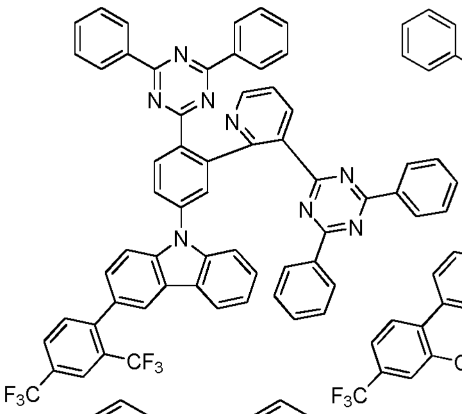
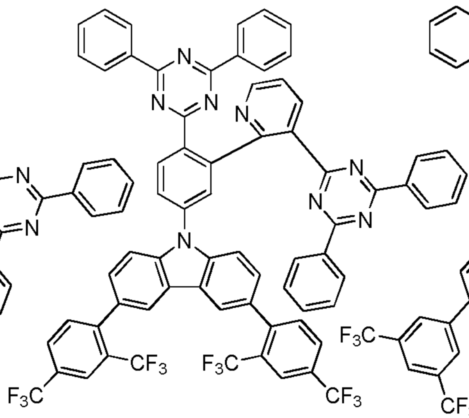
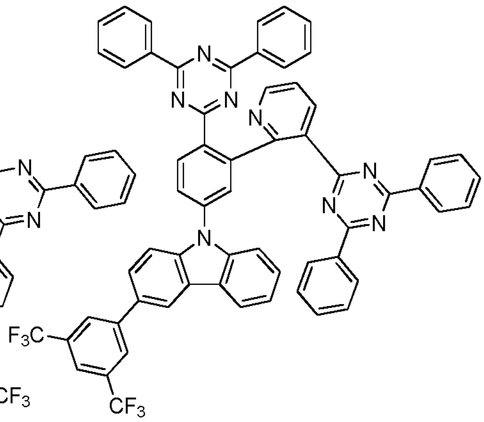
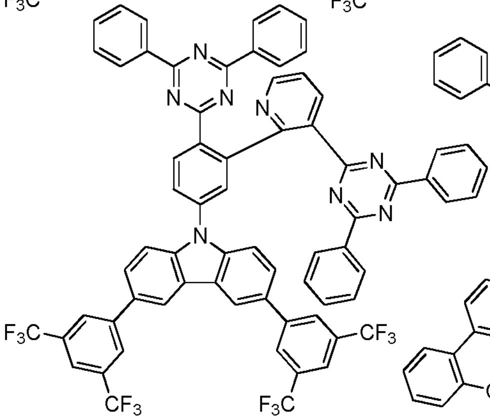
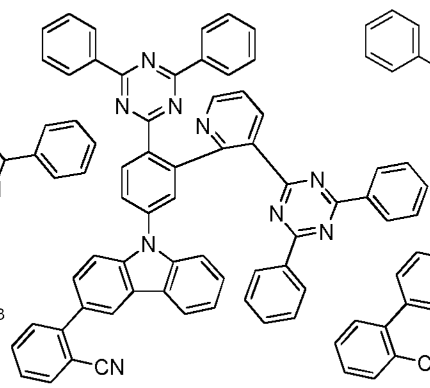
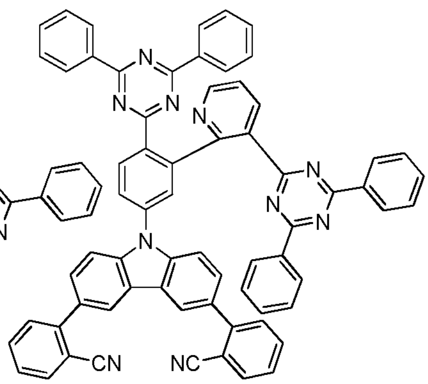
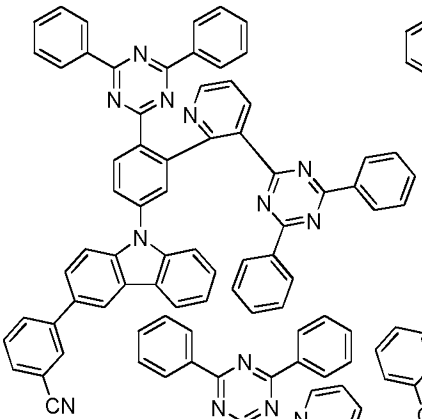
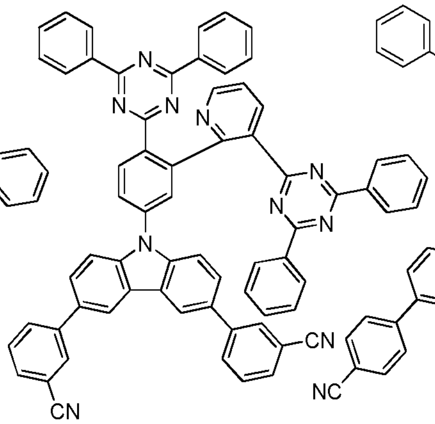
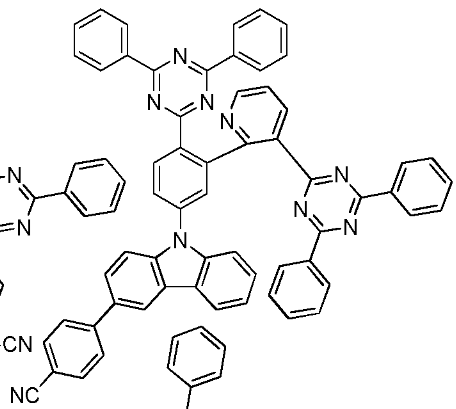
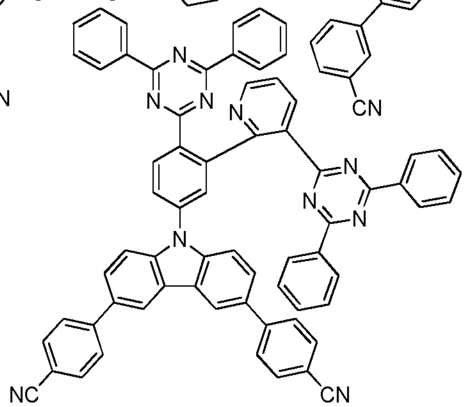
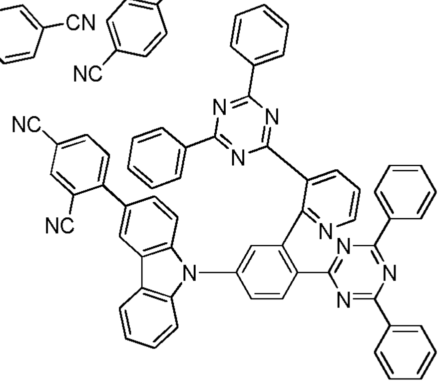


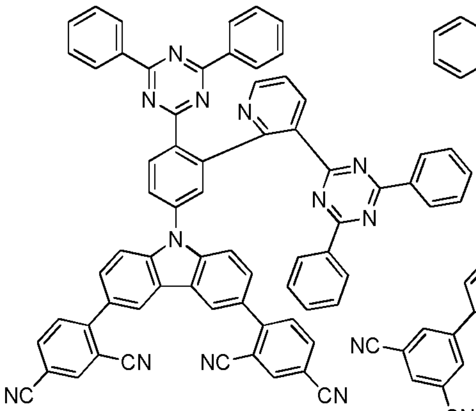
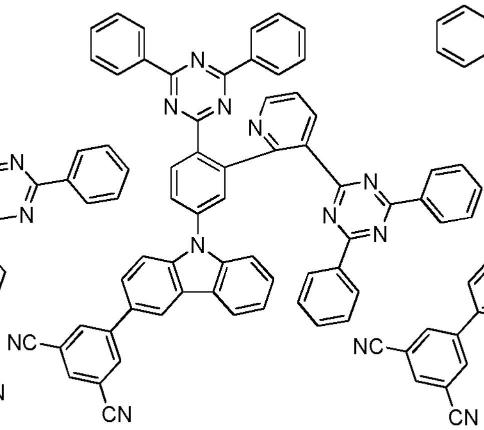
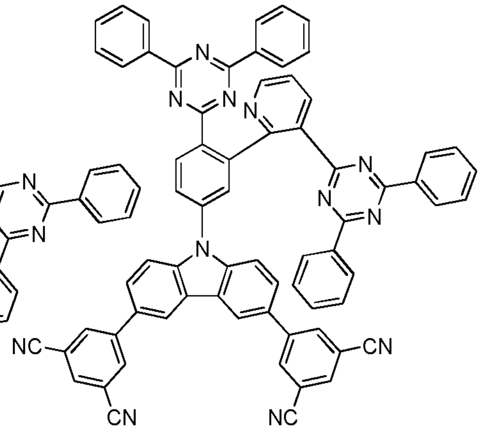
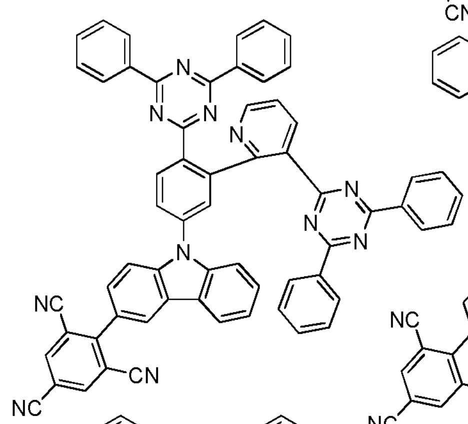
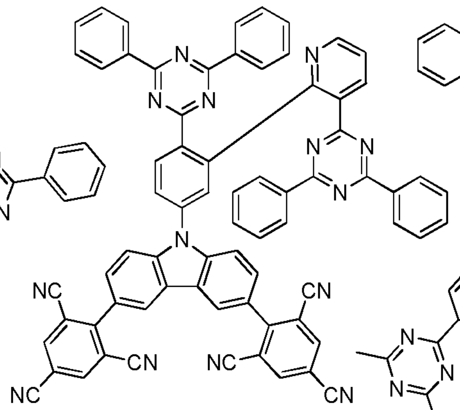
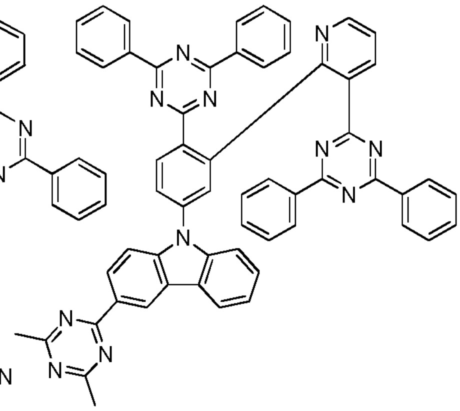
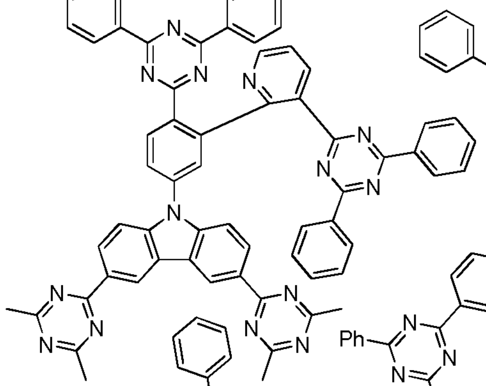
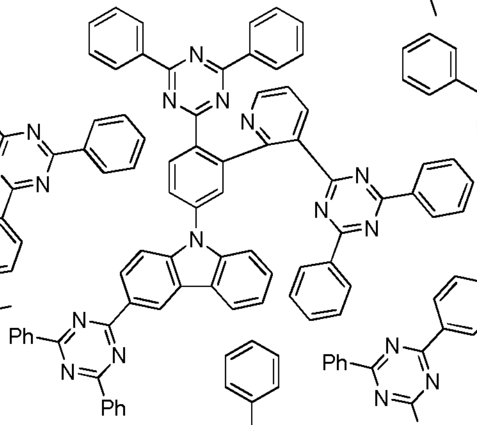
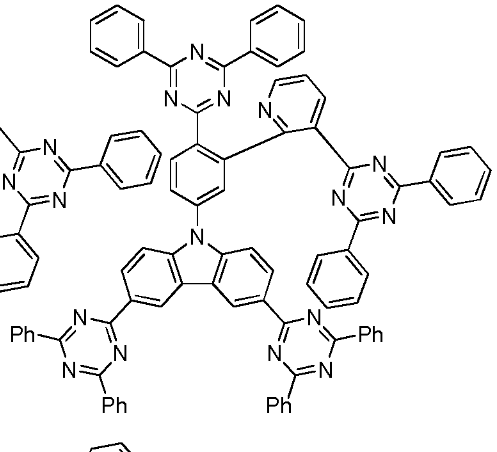
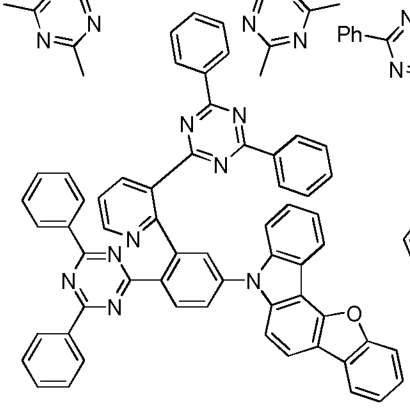
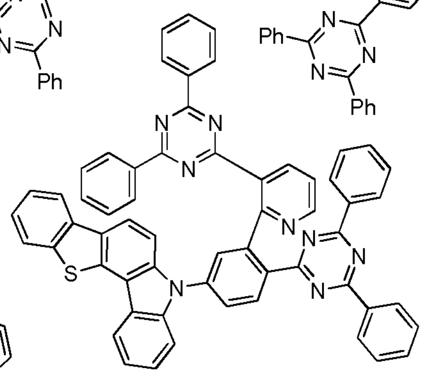


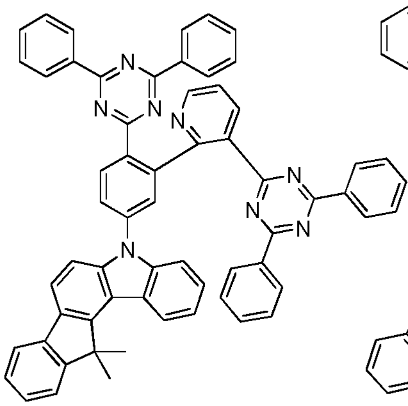
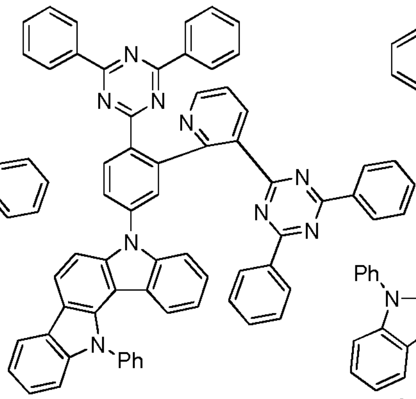
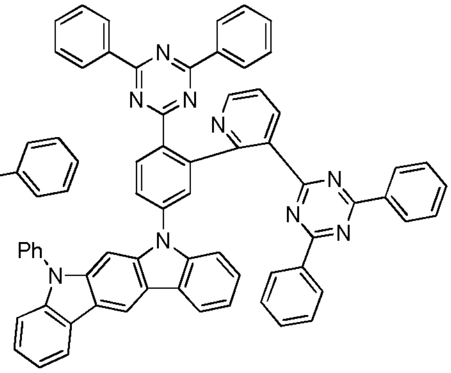
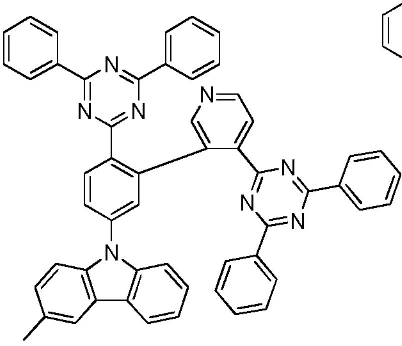
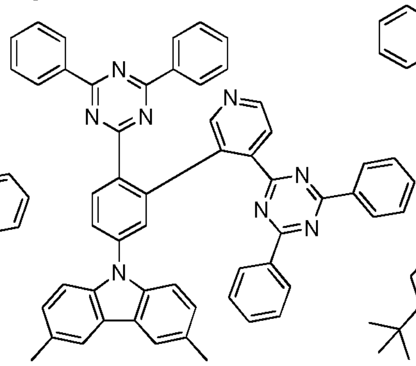
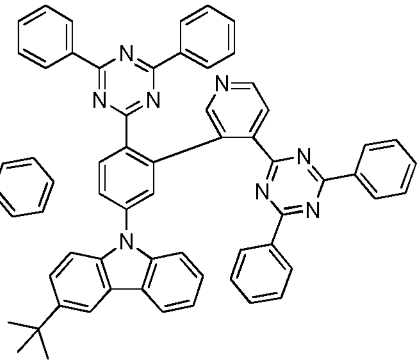
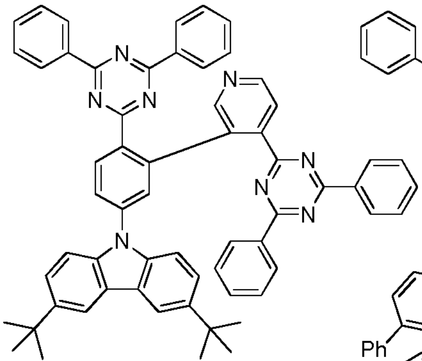
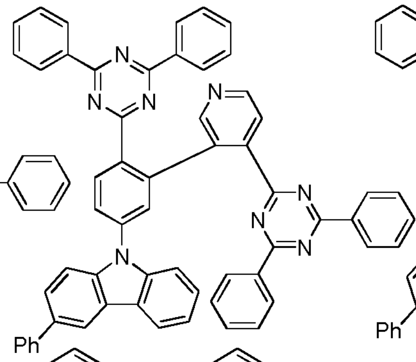
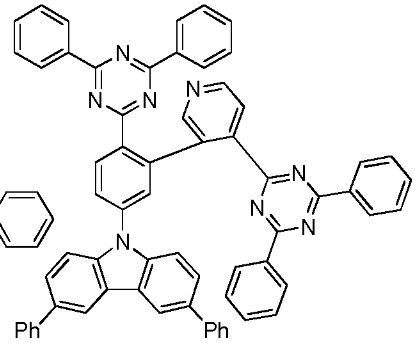
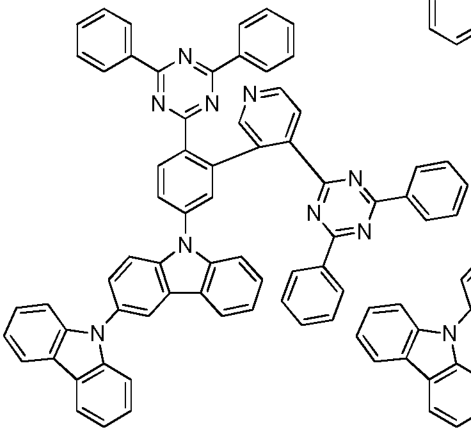
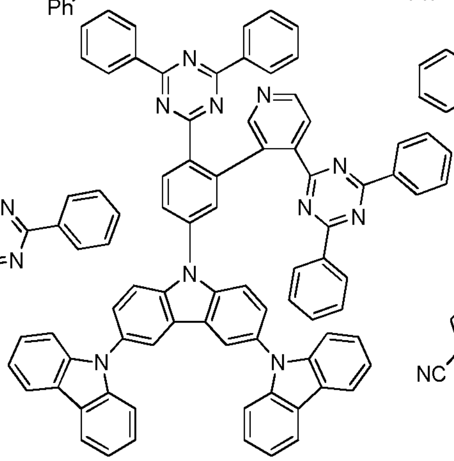
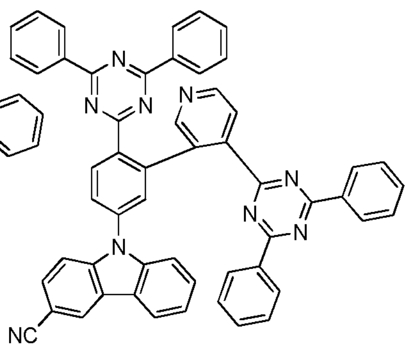


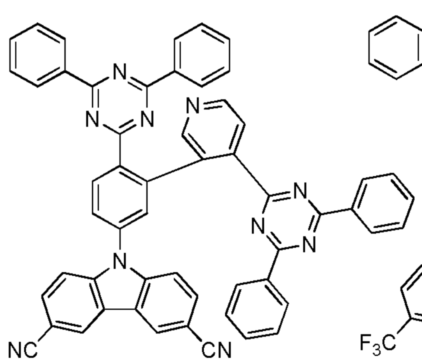
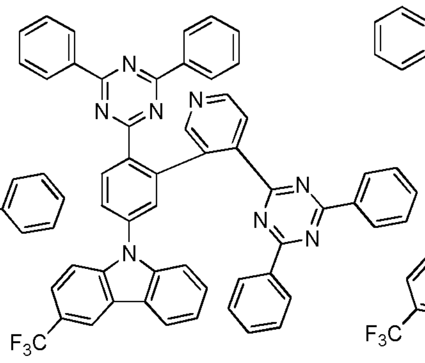
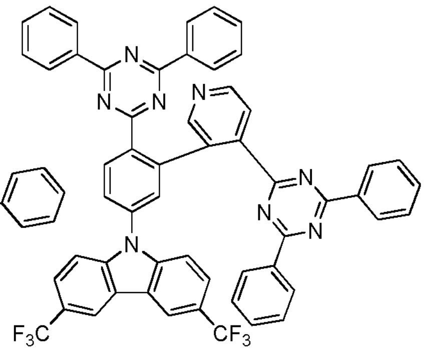
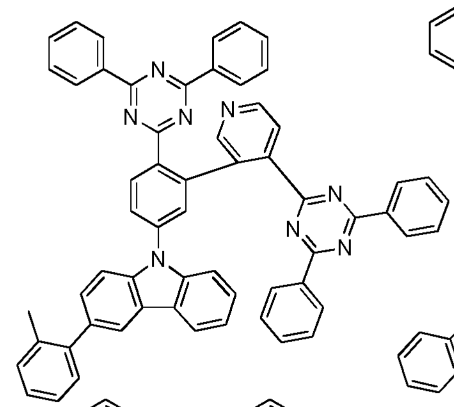
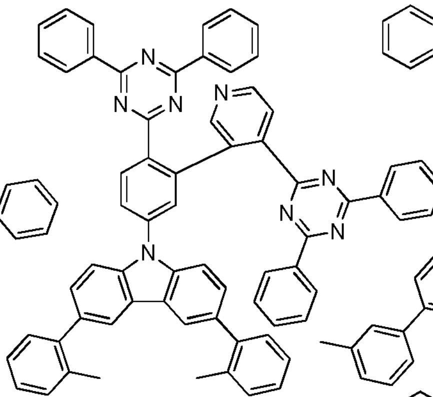
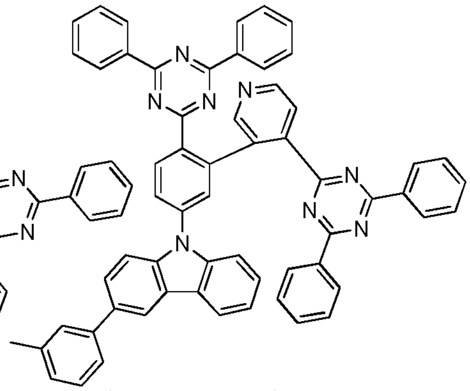
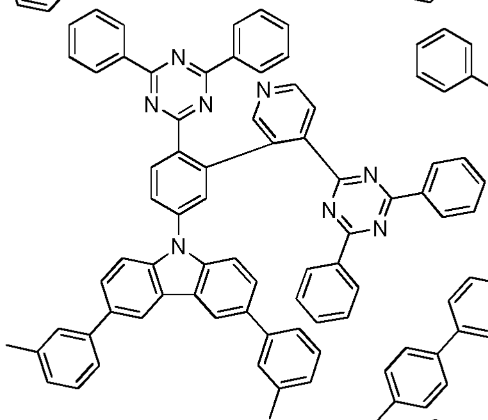
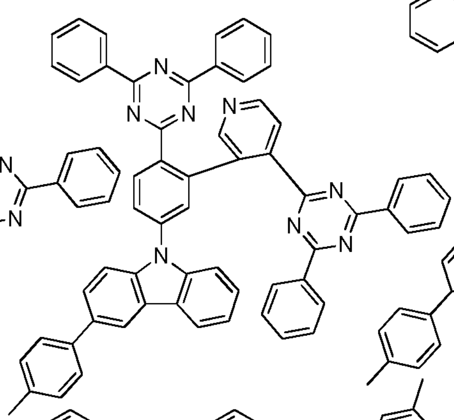
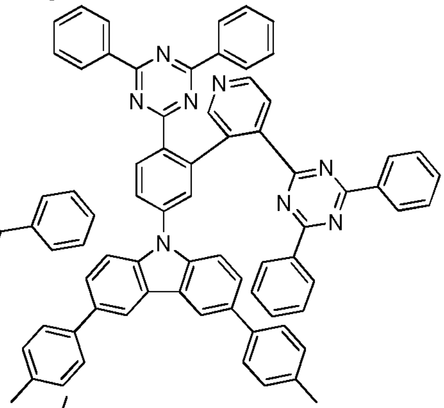
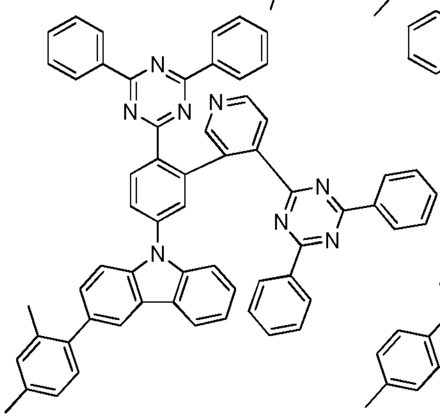
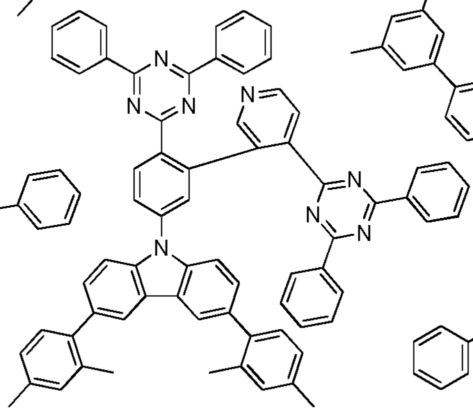
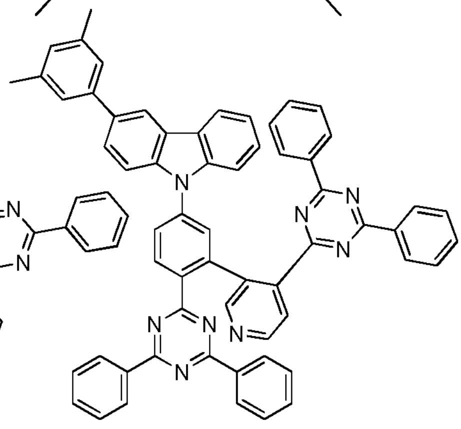


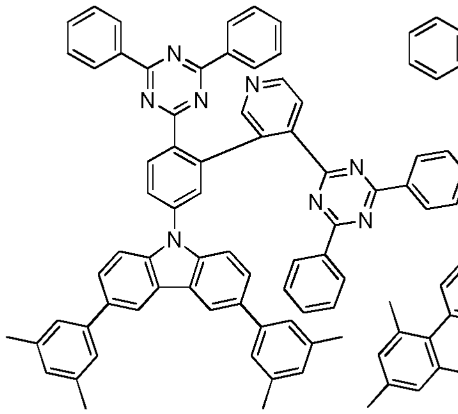
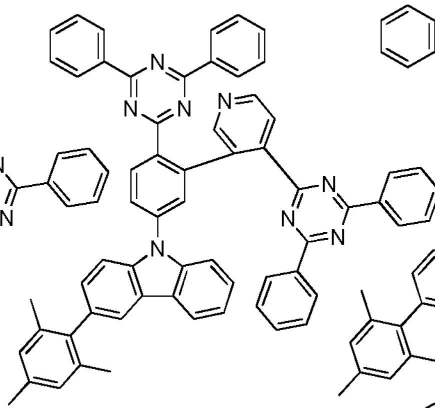
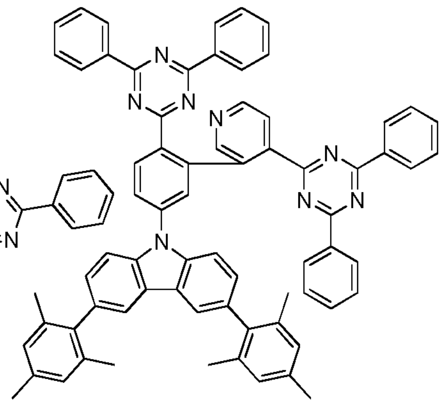
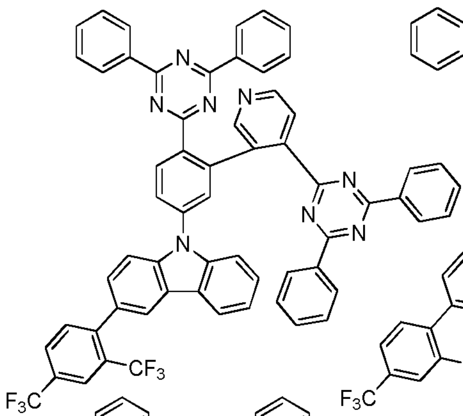
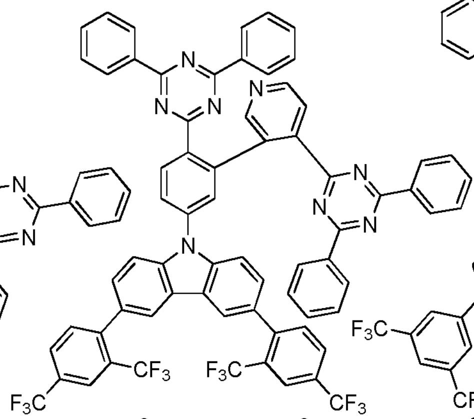
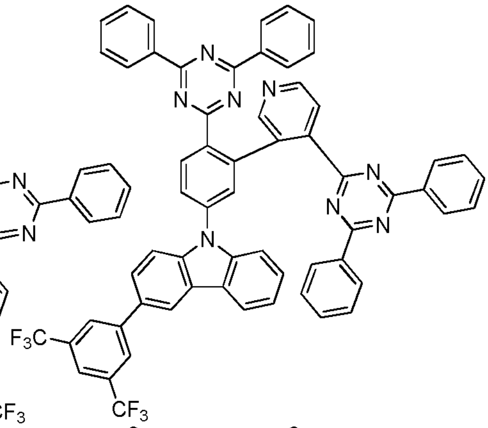
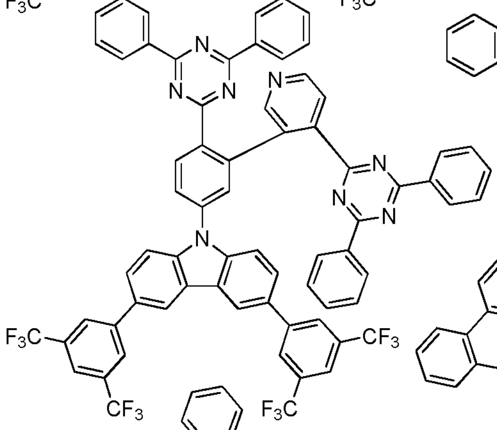
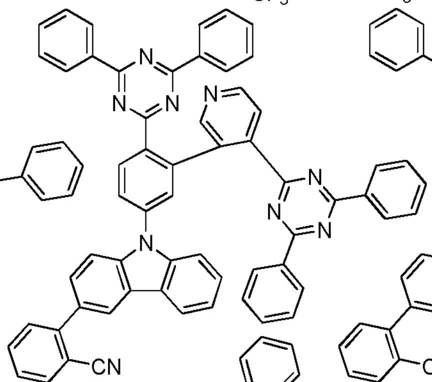
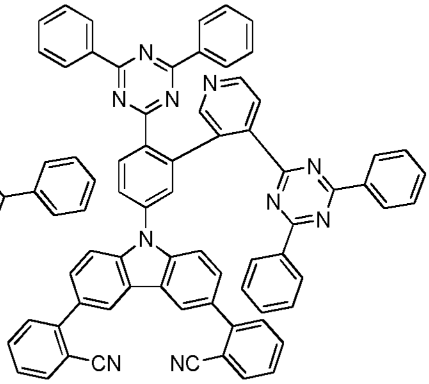
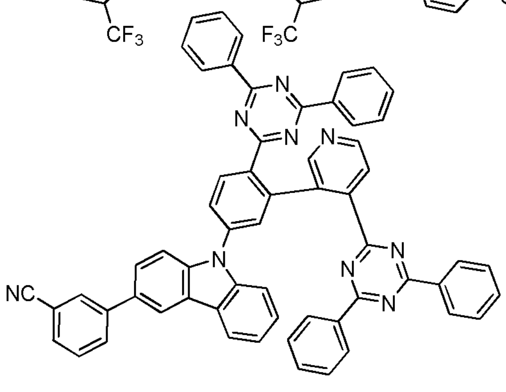
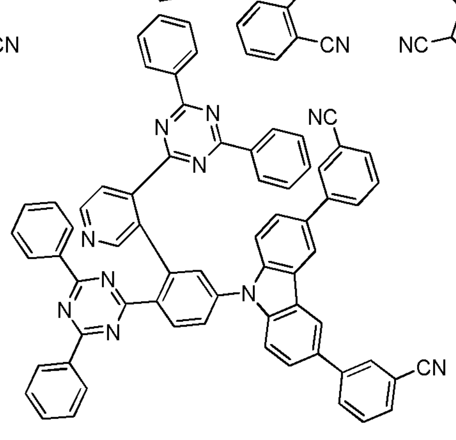













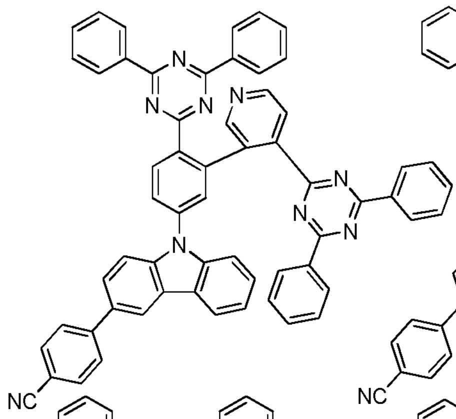
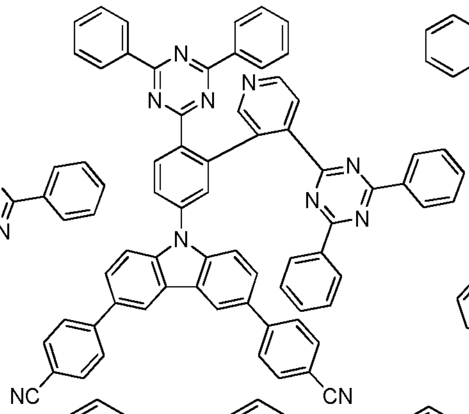
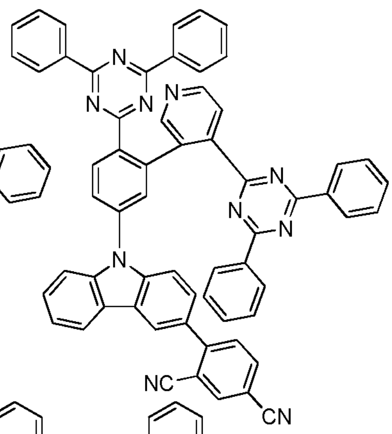
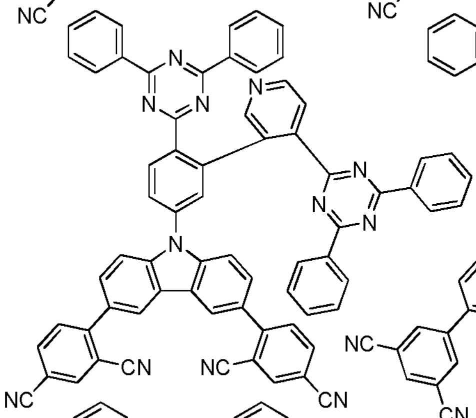
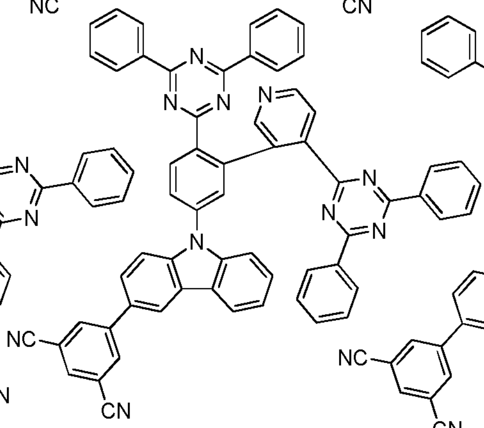
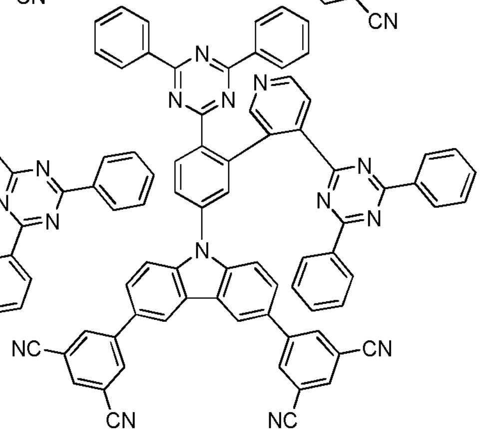
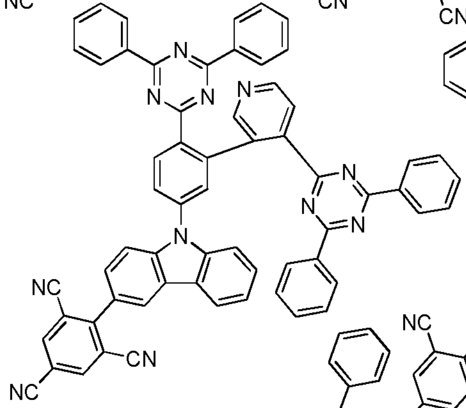
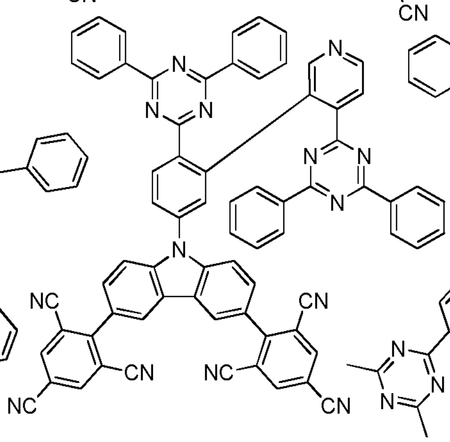
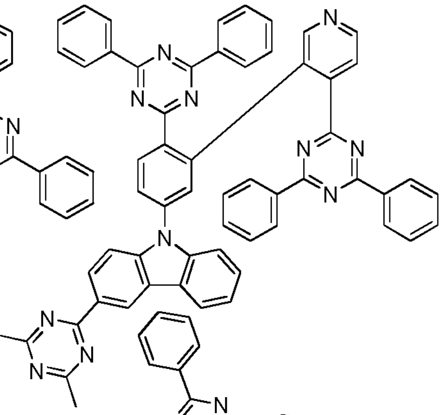
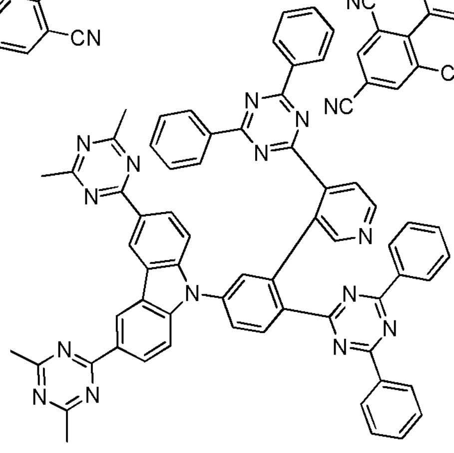
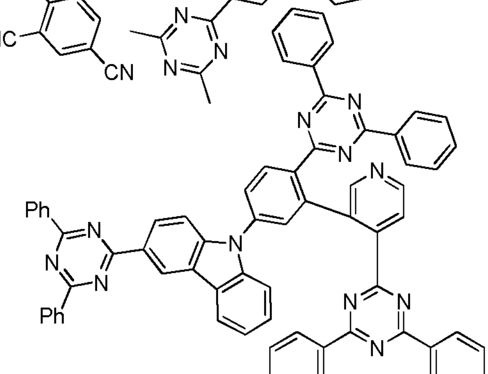












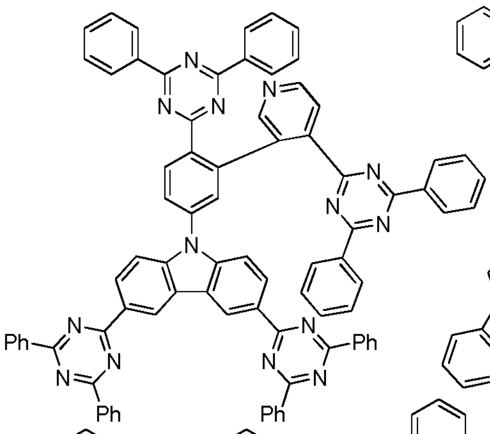
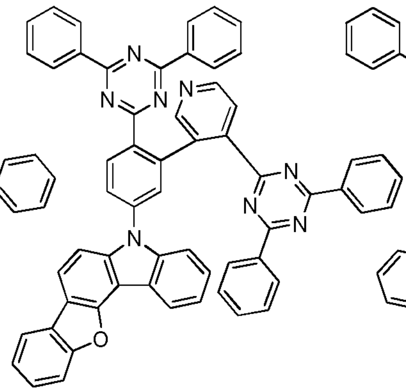
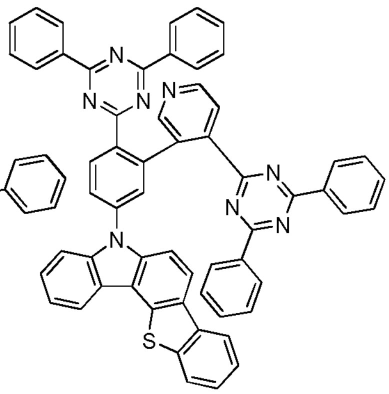
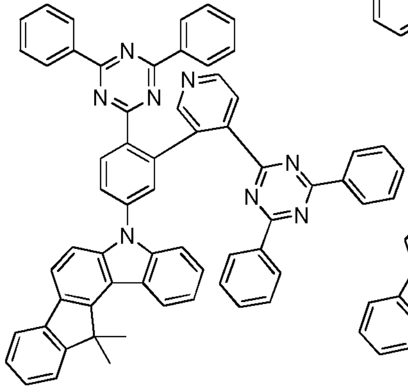
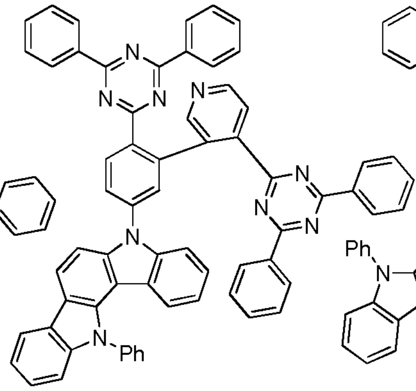
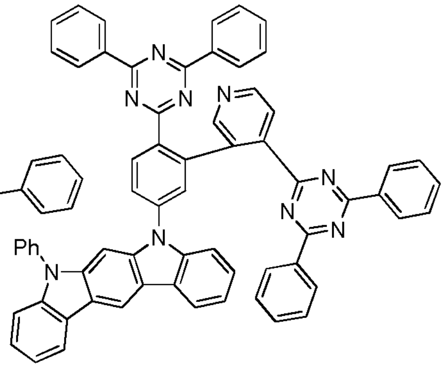
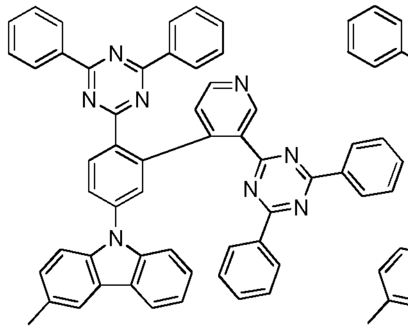
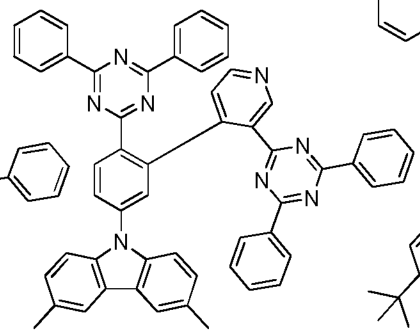
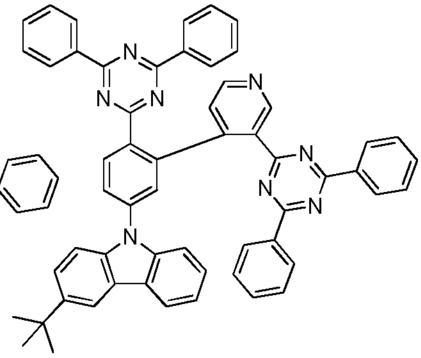
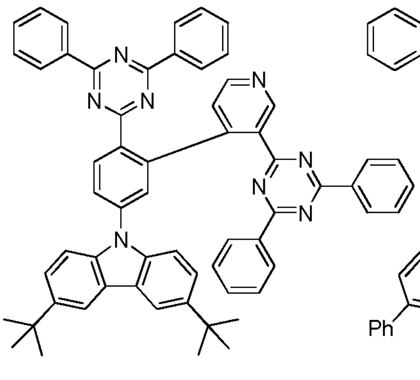
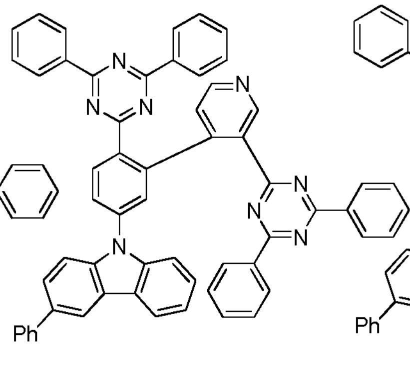
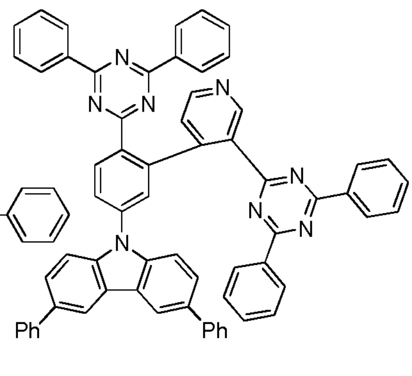












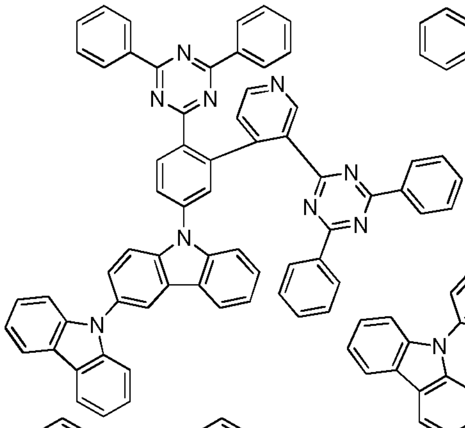
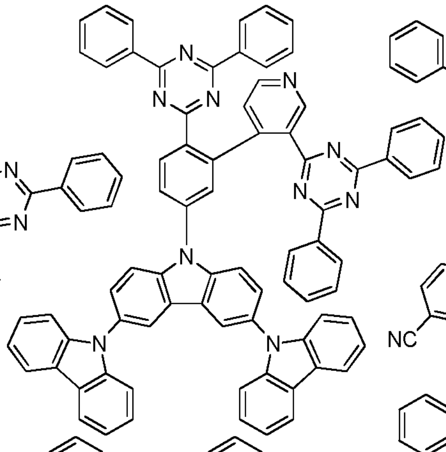
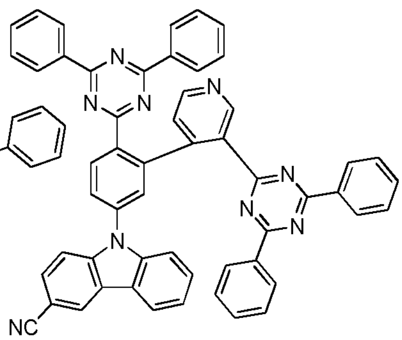
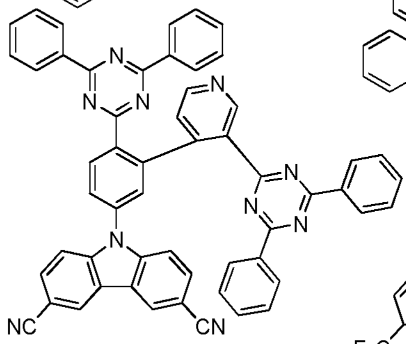
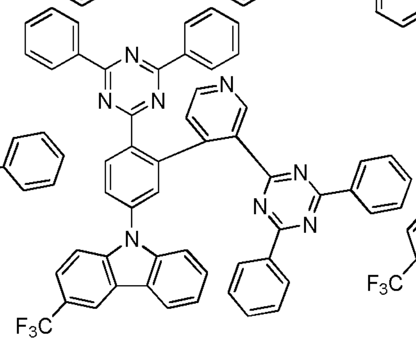
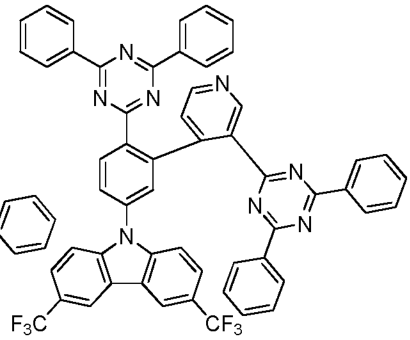
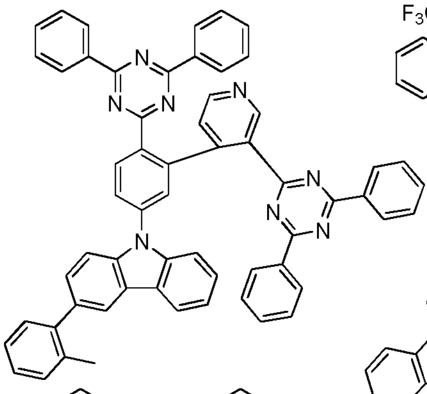
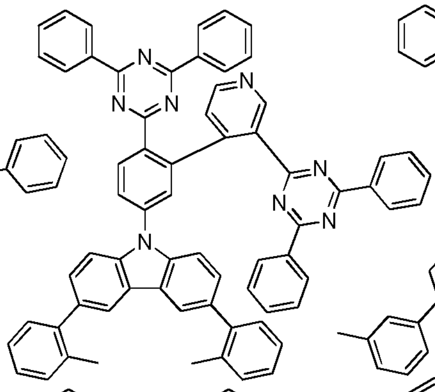
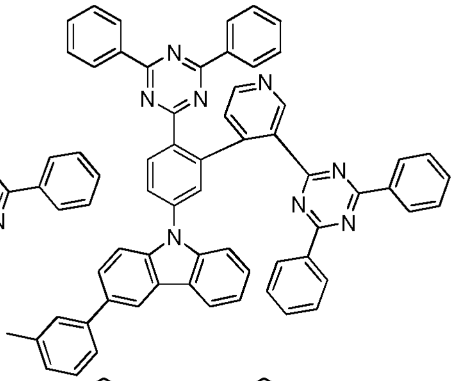
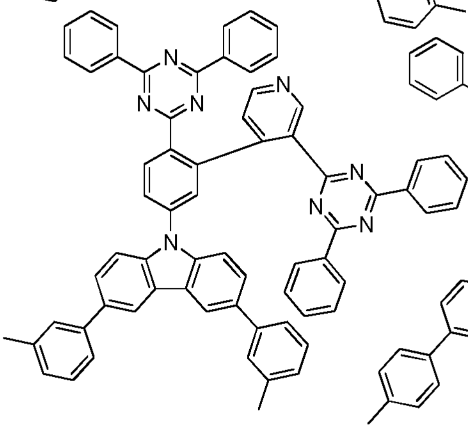
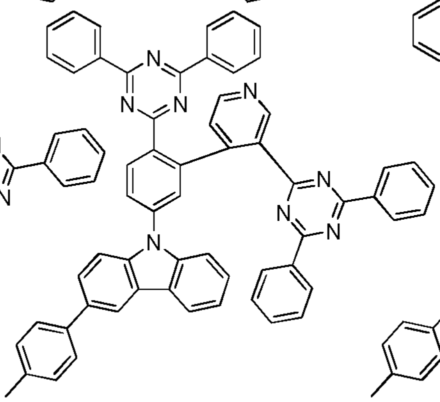
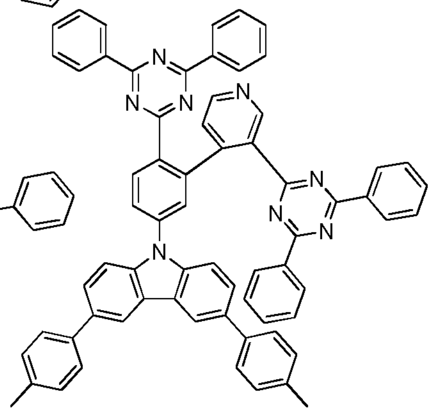













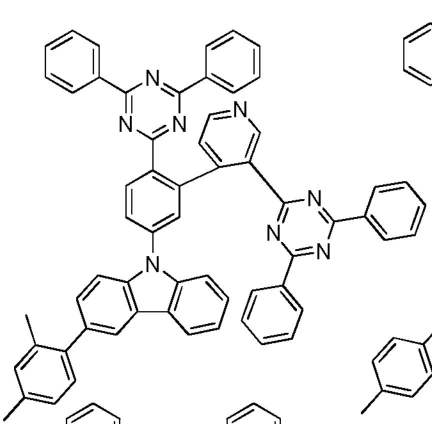
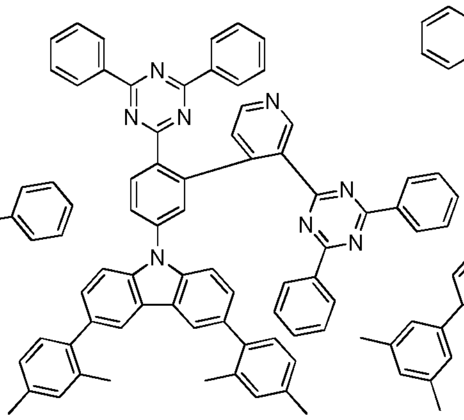
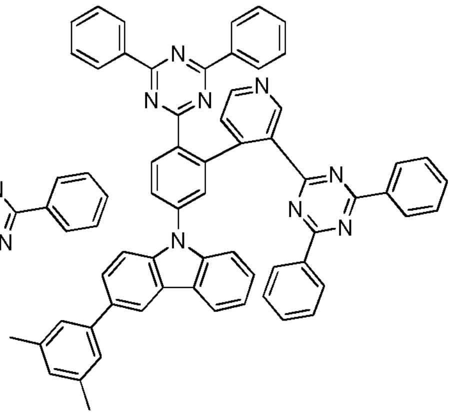
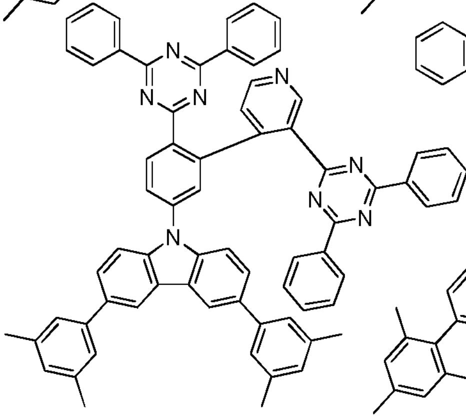
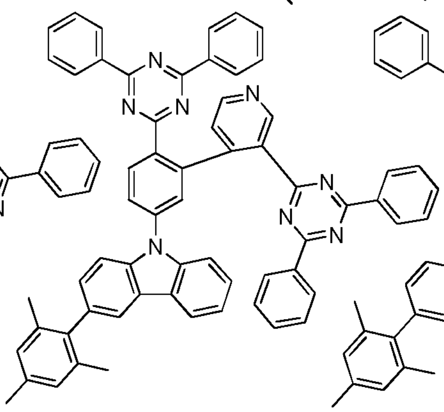
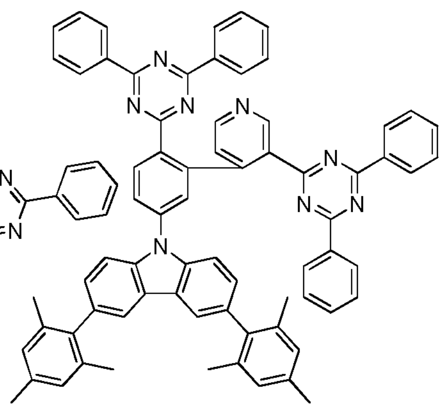
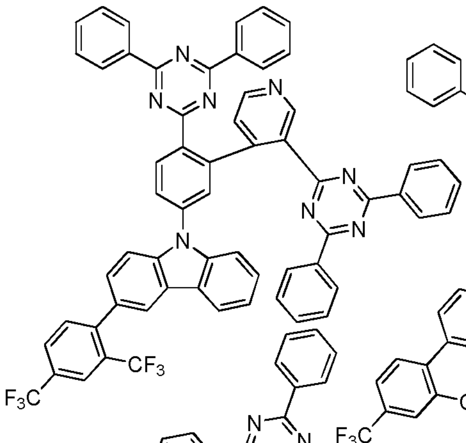
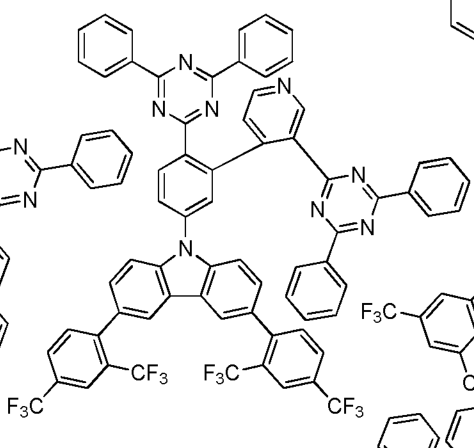
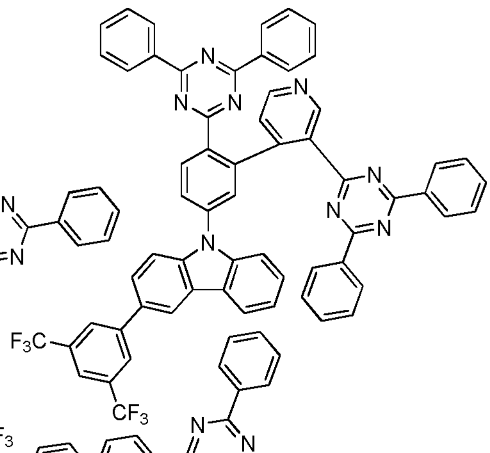
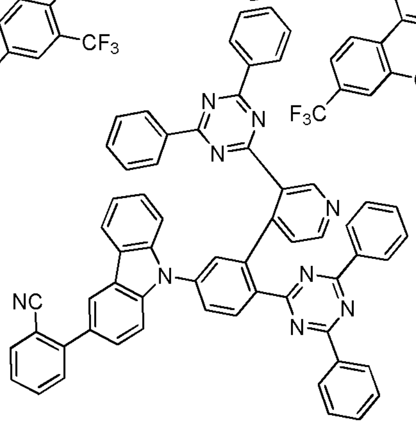
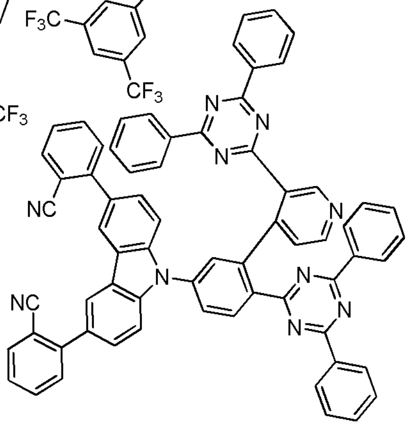













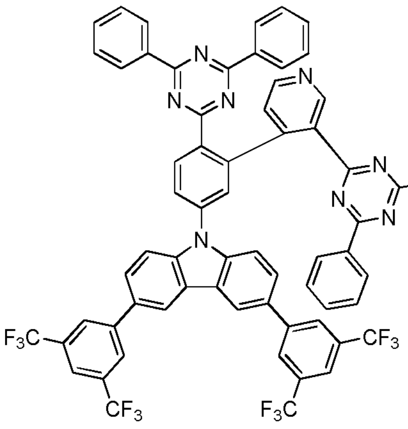
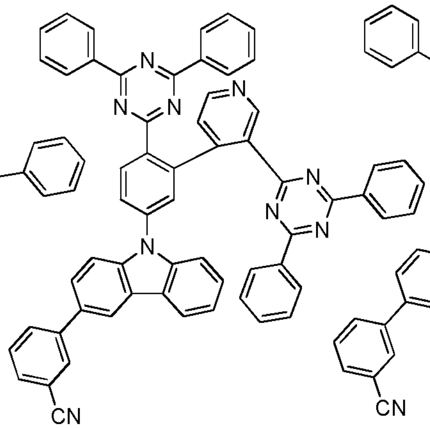
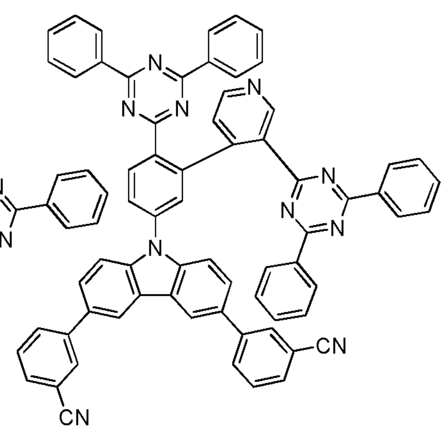












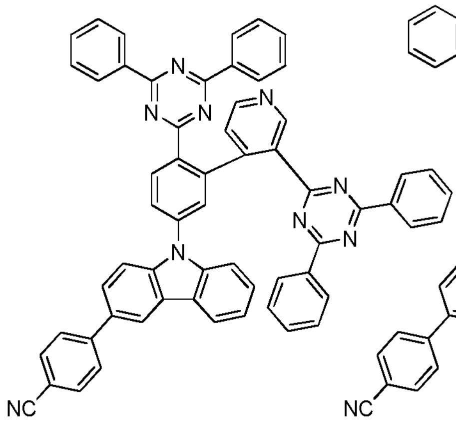
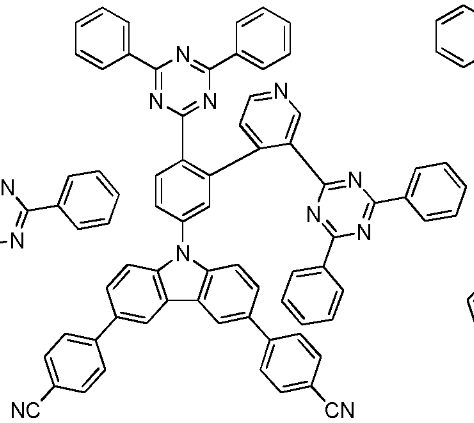
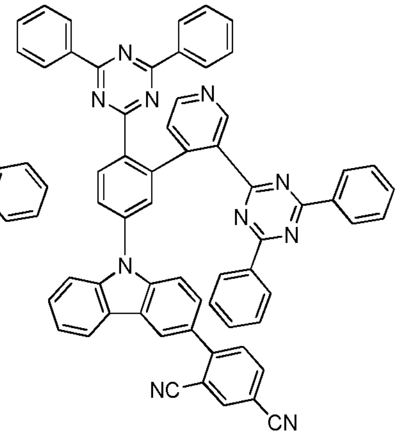












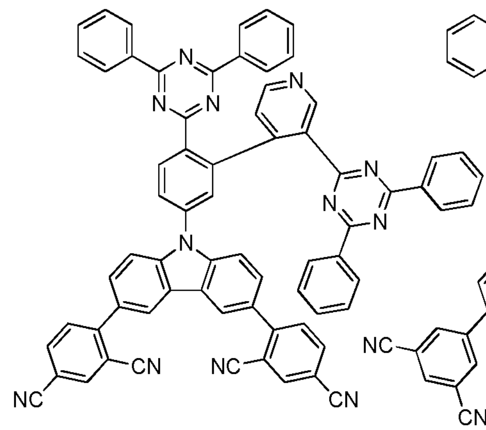
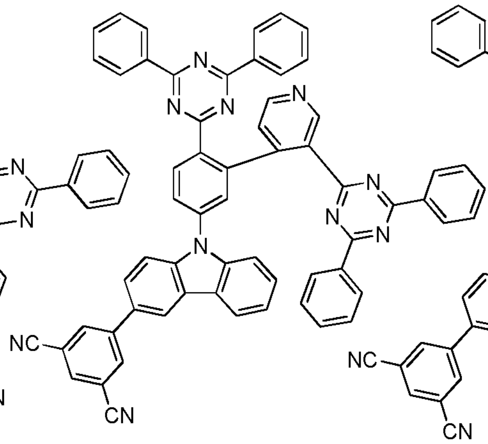
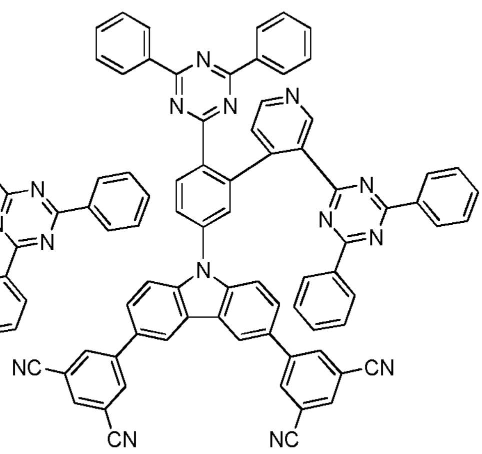













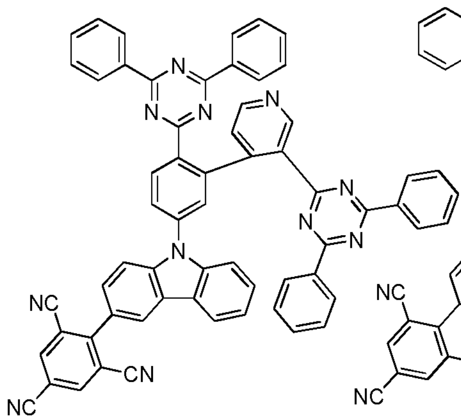













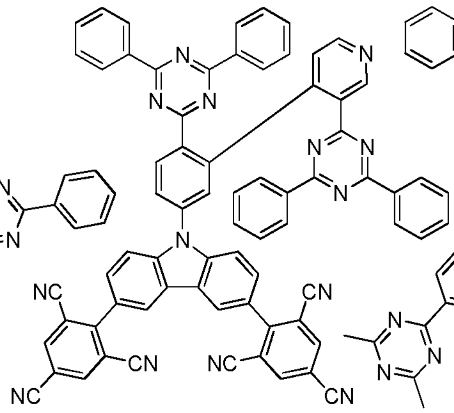












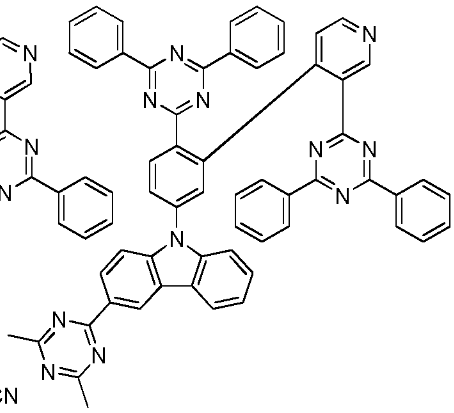




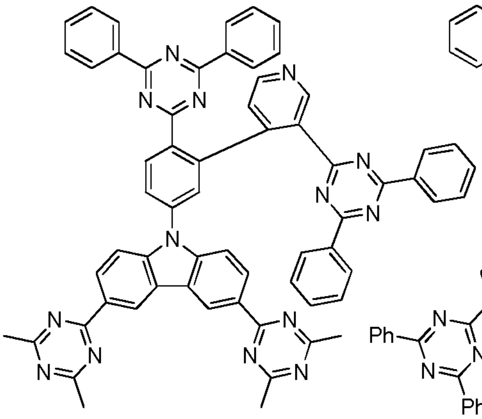




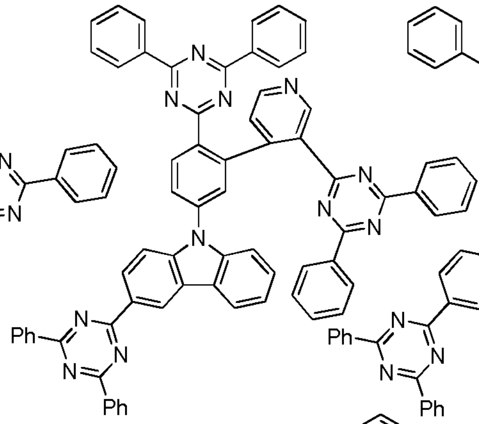




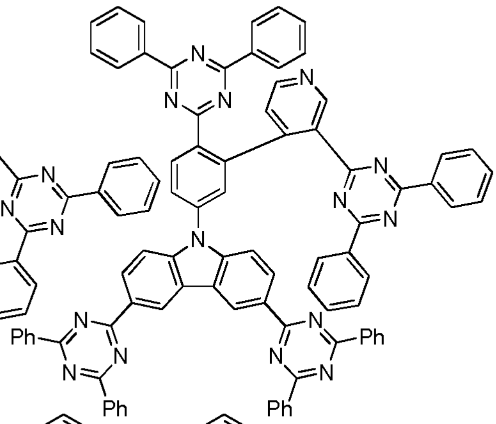


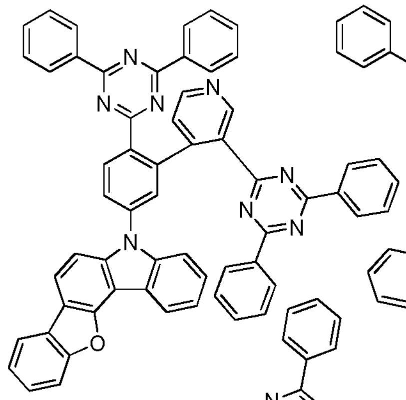


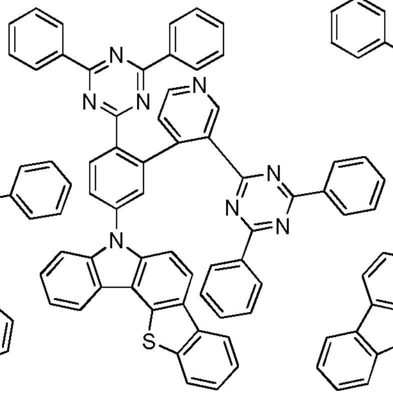


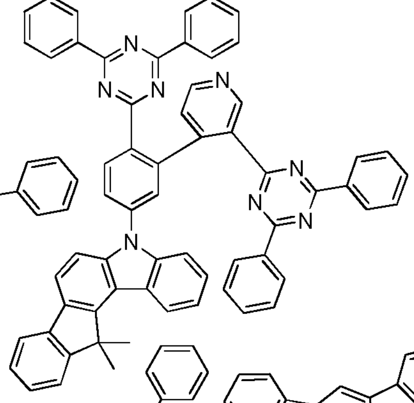


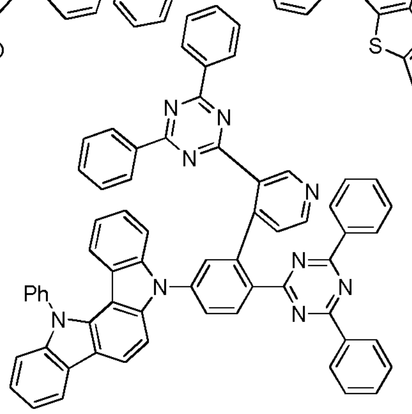


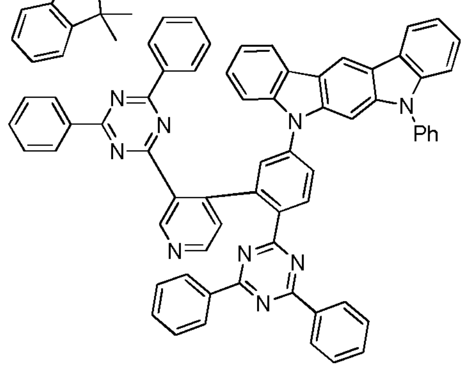












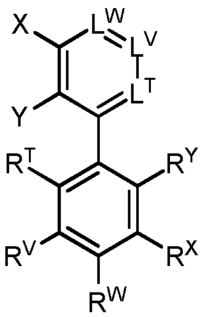
Figures

Figure 1 Emission spectrum of example **1** (10% by weight) in PMMA.

Figure 2 Emission spectrum of example **2** (10% by weight) in PMMA.

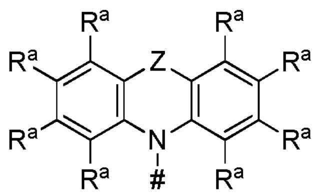
Claims

1. An organic molecule, comprising
- a first chemical moiety comprising a structure of Formula I,



Formula I

and
- one second chemical moiety comprising a structure of Formula II,



Formula II

wherein the first chemical moiety is linked to the second chemical moiety via a single bond;

wherein
L^T is N or C-T;
L^V is N or C-V;
L^W is N or C-W;

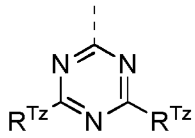
T is selected from the group consisting of R^A and R^1;
V is selected from the group consisting of R^A and R^1;
W is selected from the group consisting of R^A and R^1;
X is selected from the group consisting of R^A and R^2;
Y is selected from the group consisting of R^A and R^2;

R^T is selected from the group consisting of R^A and R^I;
R^V is selected from the group consisting of R^A and R^I;
R^W is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I;

R^X is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I;

R^Y is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I;

R^A comprises a structure of Formula Tz:



Formula Tz

wherein the dotted bond represents the binding site of R^A to the single bond linking the first chemical moiety and R^A;

represents the binding site of a single bond linking the second chemical moiety to the first chemical moiety;

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

R^1 is independently from each other at each occurrence independently from another selected from the group consisting of:

hydrogen, deuterium,

C_1-C_5-alkyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_2-C_8-alkenyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_2-C_8-alkynyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium; and

C_6-C_{18}-aryl,

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

R^2 is independently from each other at each occurrence independently from another selected from the group consisting of:

hydrogen, deuterium,

C_1-C_5-alkyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_2-C_8-alkenyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_2-C_8-alkynyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium; and

C_6-C_{18}-aryl,

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

R^I is independently from each other at each occurrence independently from another selected from the group consisting of:

hydrogen, deuterium,

C_1-C_5-alkyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_2-C_8-alkenyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_2-C_8-alkynyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium; and

C_6-C_{18}-aryl,

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

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

hydrogen, deuterium,

C_1-C_5-alkyl,

wherein one or more hydrogen atoms are optionally substituted by deuterium;

C_6-C_{18}-aryl,

which is optionally substituted with one or more substituents R^6, and

C_3-C_{17}-heteroaryl,

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

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

C_1-C_{40}-alkyl,

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

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

C_1-C_{40}-alkoxy,

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

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

C_1-C_{40}-thioalkoxy,

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

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

C_2-C_{40}-alkenyl,

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

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

C_2-C_{40}-alkynyl,

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

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

C_6-C_{60}-aryl,

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

C_3-C_{57}-heteroaryl,

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

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

C_1-C_{40}-alkyl,

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

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

C_1-C_{40}-alkoxy,

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

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

C_1-C_{40}-thioalkoxy,

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

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

C_2-C_{40}-alkenyl,

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

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

C_2-C_{40}-alkynyl,

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

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

C_6-C_{60}-aryl,

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

C_3-C_{57}-heteroaryl,

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

R^6 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 one or more hydrogen atoms are optionally, independently from each other substituted by deuterium, CN, CF_3, or F;

C_1-C_5-alkoxy,

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

C_1-C_5-thioalkoxy,

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

C_2-C_5-alkenyl,

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

C_2-C_5-alkynyl,

wherein one or more hydrogen atoms are optionally, 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$)_2$;

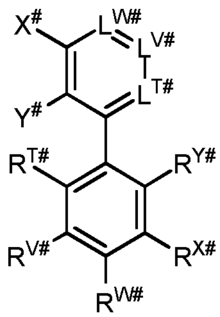
$N(C_3$-C_{17}-heteroaryl$)_2$,

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

wherein the substituents R^a, R^3, R^4 or R^5 independently from each other optionally form a mono- or polycyclic, aliphatic, aromatic and/or benzo-fused ring system with one or more substituents R^a, R^3, R^4 or R^5;

wherein
- exactly one ring member (atom or group) selected from the group consisting of L^T, L^V and L^W is N,
- exactly one substituent selected from the group consisting of R^T, R^V, R^W, R^X and R^Y is R^A,
- exactly one substituent selected from the group consisting of T, V, W, X and Y is R^A, and
- exactly one substituent selected from the group consisting of R^W, R^Y and R^X represents the binding site of a single bond linking the first chemical moiety and the second chemical moiety.

2. The organic molecule according to claim 1, wherein the first chemical moiety comprises a structure of Formula Ia:



Formula Ia

wherein
$L^{T\#}$ is N or C-R^1;
$L^{V\#}$ is N or C- R^1,
$L^{W\#}$ is N or C-$W^\#$;
$W^\#$ is selected from the group consisting of R^A and R^1;
$X^\#$ is selected from the group consisting of R^A and R^2;
$Y^\#$ is selected from the group consisting of R^A and R^2;
$R^{T\#}$ is selected from the group consisting of R^A and R^I;
$R^{V\#}$ is selected from the group consisting of R^A and R^I;
$R^{W\#}$ is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is selected from the group consisting of R^A and R^I;
$R^{X\#}$ is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is R^I;

$R^{Y\#}$ is the binding site of a single bond linking the first chemical moiety to the second chemical moiety or is R^{I};

wherein exactly one ring member (atom or group) selected from the group consisting of $L^{T\#}$, $L^{V\#}$ and $L^{W\#}$ is N;

exactly one substituent selected from the group consisting of $R^{T\#}$, $R^{V\#}$ and $R^{W\#}$ is R^{A};

exactly one substituent selected from the group consisting of $W^{\#}$, $X^{\#}$ and $Y^{\#}$ is R^{A}

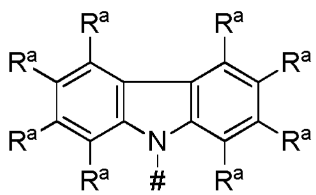
exactly one substituent selected from the group consisting of $R^{W\#}$, $R^{Y\#}$ and $R^{X\#}$ represents the binding site of a single bond linking the first chemical moiety and the second chemical moiety;

and wherein apart from that the definitions in claim 1 apply.

3. The organic molecule according to claim 1 or 2, wherein R^1, R^2 and R^I is independently from each other at each occurrence independently from another selected from the group consisting of H, methyl, mesityl, tolyl and phenyl.

4. The organic molecule according to one or more of claims 1 to 3, wherein R^{Tz} is independently from each other selected from the group consisting of H, methyl and phenyl.

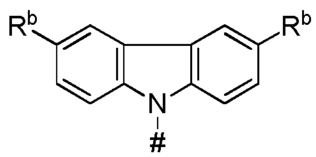
5. The organic molecule according to one or more of claims 1 to 4, wherein the second chemical moiety comprises a structure of Formula IIa:



Formula IIa

wherein # and R^a are defined as in claim 1.

6. The organic molecule according to one or more of claims 1 to 5, wherein the second chemical moiety comprises a structure of Formula IIb:



Formula IIb

wherein

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

C_1-C_{40}-alkyl,

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

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

C_1-C_{40}-alkoxy,

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

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

C_1-C_{40}-thioalkoxy,

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

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

C_2-C_{40}-alkenyl,

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

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

C_2-C_{40}-alkynyl,

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

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

C_6-C_{60}-aryl,

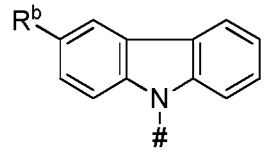
which is optionally substituted with one or more substituents R^5; and

C_3-C_{57}-heteroaryl,

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

and wherein apart from that the definitions in claim 1 apply.

7. The organic molecule according to one or more of claims 1 to 5, wherein the second chemical moiety comprises a structure of Formula IIc:



Formula IIc

wherein

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

C_1-C_{40}-alkyl,

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

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

C_1-C_{40}-alkoxy,

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

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

C_1-C_{40}-thioalkoxy,

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

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

C_2-C_{40}-alkenyl,

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

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

C_2-C_{40}-alkynyl,

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

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

C_6-C_{60}-aryl,

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

C_3-C_{57}-heteroaryl,

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

and wherein apart from that the definitions in claim 1 apply.

8. The organic molecule according to claim 6 or 7, wherein R^b is at each occurrence independently from another selected from the group consisting of

- 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

- $N(Ph)_2$.

9. Use of an organic molecule according to one or more of claims 1 to 8 as a luminescent emitter and/or a host material and/or an electron transport material and/or a hole injection material and/or a hole blocking material in an optoelectronic device.

10. The use according to claim 9, 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.

11. A composition, comprising:

(a) at least one organic molecule according to one or more of claims 1 to 8, 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 8, and

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

12. An optoelectronic device, comprising an organic molecule according to one or more of claims 1 to 8 or a composition according to claim 11, 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.

13. The optoelectronic device according to claim 12, comprising
- 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 the anode and the cathode and which comprises an organic molecule according to one or more of claims 1 to 8 or a composition according to claim 11.

14. A method for producing an optoelectronic device, wherein an organic molecule according to any of claims 1 to 8 or a composition according to claim 11 is used.

15. The method according to claim 14, comprising processing the organic molecule by a vacuum evaporation method or from a solution.

Figure 1

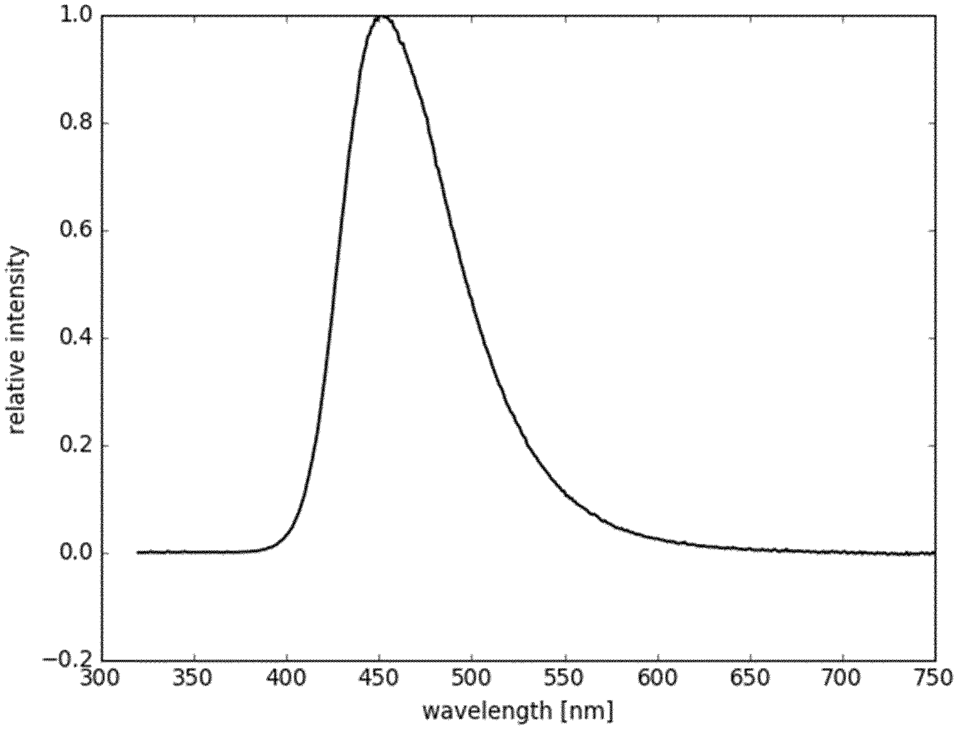
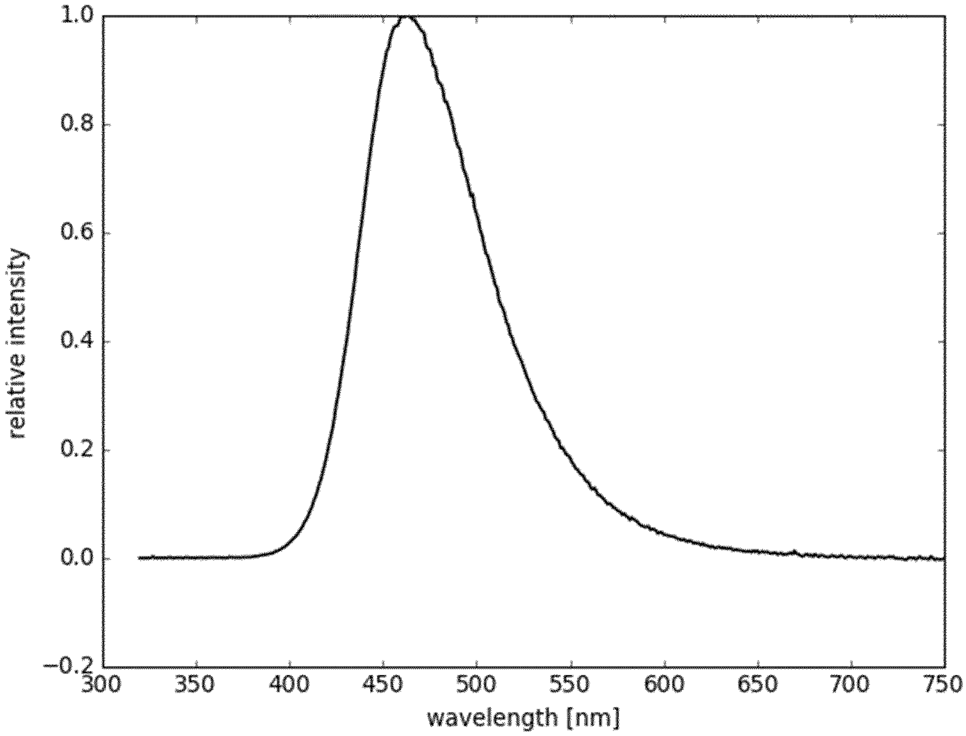


Figure 2



INTERNATIONAL SEARCH REPORT

International application No
PCT/EP2018/084183

A. CLASSIFICATION OF SUBJECT MATTER
INV. C07D401/14 C07D487/04 C07D491/048 C07D495/04 H01L51/00 C09K11/07
ADD.

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

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
C07D H01L

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

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

EPO-Internal, WPI Data, CHEM ABS Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 2016/159479 A1 (INDUSTRY-ACADEMIC COOPERATION FOUNDATION DANKOOK UNIV [KR]) 6 October 2016 (2016-10-06) claims page 29; compound 1 page 36; compound 45 -----	1-15
A	WO 2012/108879 A1 (UNIVERSAL DISPLAY CORP [US]; IDEMITSU KOSAN CO [JP]; YAMAMOTO HITOSHI) 16 August 2012 (2012-08-16) claim 10 -----	1-15
A	US 2015/318510 A1 (ITO NAOYUKI [KR] ET AL) 5 November 2015 (2015-11-05) page 127 -----	1-15

☐ Further documents are listed in the continuation of Box C.

☒ See patent family annex.

* Special categories of cited documents :

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"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

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"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
11 March 2019	21/03/2019

Name and mailing address of the ISA/	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Bedel, Christian

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/EP2018/084183

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
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		EP 3275968 A1	31-01-2018
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