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경기도 성남시 중원구 갈마치로 176
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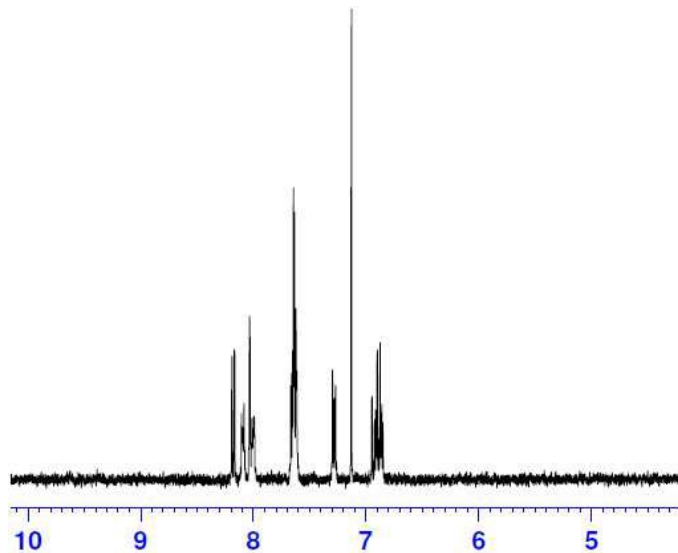
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(57) 요약

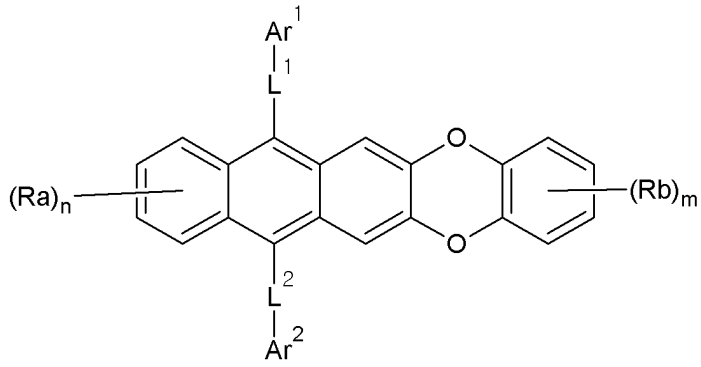
하기 화학식 1로 표시되는 유기 발광 화합물이 제공된다.

(뒷면에 계속)

대표도 - 도1



<화학식 1>



상기 식에서, Ar^1 , Ar^2 , L^1 , L^2 , Ra, Rb, n 및 m은 전술하여 정의된 바와 같다.

(72) 발명자

안도환

경기도 성남시 중원구 갈마치로 176

이대균

경기도 성남시 중원구 갈마치로 176

김소연

경기도 성남시 중원구 갈마치로 176

오민영

경기도 성남시 중원구 갈마치로 176

안준수

경기도 성남시 중원구 갈마치로 176

신정철

경기도 성남시 중원구 갈마치로 176

임현철

경기도 성남시 중원구 갈마치로 176

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안중복

경기도 성남시 중원구 갈마치로 176

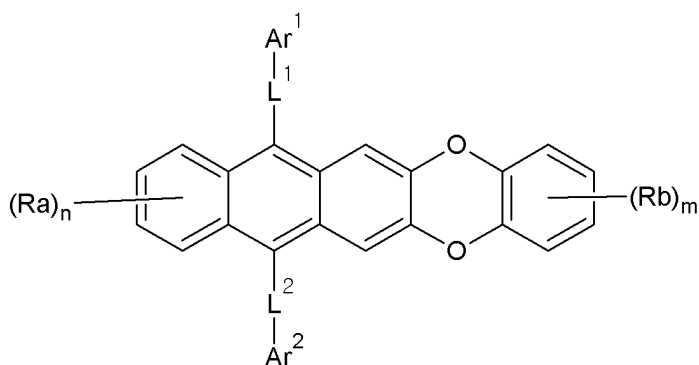
명세서

청구범위

청구항 1

하기 화학식 1로 표시되는 유기 발광 화합물:

<화학식 1>



상기 식에서,

Ar^1 및 Ar^2 는, 각각 독립적으로, 치환 또는 비치환된 C6-C60의 아릴기 또는 치환 또는 비치환된 C3-C60의 헤테로아릴기이고,

상기 Ar^1 및 Ar^2 이 치환된 경우의 치환기는 중수소, 불소, C1-C30의 알킬기, C6-C30의 아릴기, C2-C30의 헤테로아릴기, C1-C30의 알콕시기, C1-C30의 플루오로알킬기, $-Si(CH_3)_3$ 및 $-CN$ 로 이루어진 군에서 선택된 하나이고;

L^1 및 L^2 는, 각각 독립적으로, 단일 결합, 치환 또는 비치환된 C6-C60의 아릴렌기, 치환 또는 비치환된 C3-C60의 헤테로아릴렌기, 치환 또는 비치환된 C3-C60의 시클로알킬렌기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬렌기 및 이들의 조합으로 이루어진 군으로부터 선택된 하나이고,

상기 L^1 및 L^2 이 치환된 경우의 치환기는 C1-C20의 알킬기 및 C3-C20의 아릴기로 이루어진 군에서 선택된 적어도 하나이고;

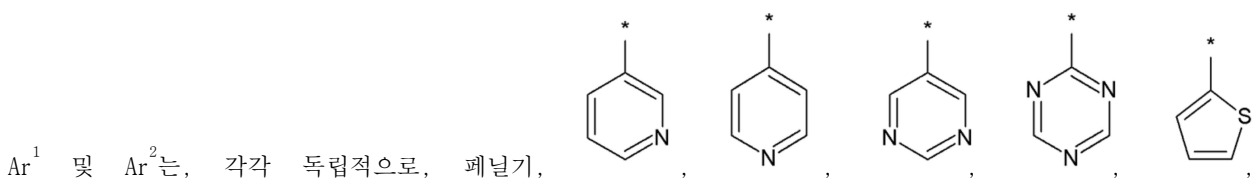
Ra 및 Rb는, 각각 독립적으로, 치환 또는 비치환된 C6-C60의 아릴기, 치환 또는 비치환된 C3-C60의 헤테로아릴기, 치환 또는 비치환된 C3-C60의 시클로알킬기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬기, $-N(R1)(R2)$, $-P(O)(R3)(R4)$ 또는 $-Si(R5)(R6)(R7)$ 이고, 상기 R1, R2, R3, R4, R5, R6 및 R7은, 각각 독립적으로, C6-C50의 아릴기 또는 C3-C50의 헤테로아릴기이고,

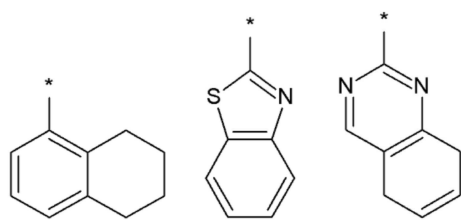
상기 Ra 및 Rb가 치환된 경우의 치환기는 C1-C30의 알킬기 또는 C1-C30의 알콕시기이고;

n 및 m은, 각각 독립적으로, 0 내지 4의 정수이다.

청구항 2

제1항에 있어서,

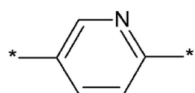




, , , 3원 내지 6원환의 고리가 2 내지 5개 융합되거나, 축합되거나 또는 스피로 구조로 연결된 C6-C60의 고리기 및 이들의 조합으로 이루어진 군으로부터 선택된 하나이고, 상기 3원 내지 6원환의 고리는 방향족고리이며 헤테로원자를 포함하거나 포함하지 않을 수 있고,

상기 정의된 Ar^1 및 Ar^2 중 수소 원자는 C1-C30 알킬기 또는 C6-C30 아릴기로 치환 또는 비치환되고;

L^1 및 L^2 는, 각각 독립적으로, 단일 결합, 비페닐렌, C1-C20 알킬기 또는 332]로 치환 또는 비치환된 페닐렌기,



, 또는 3원 내지 6원환의 고리가 2 내지 5개 융합되거나, 축합되거나 또는 스피로 구조로 연결된 C6-C60의 2가 고리기이고, 상기 3원 내지 6원환의 고리는 지환족 또는 방향족 고리일 수 있으며 헤테로원자를 포함하거나 포함하지 않을 수 있고,

상기 정의된 L^1 및 L^2 중 수소 원자는 페닐기로 치환 또는 비치환되는

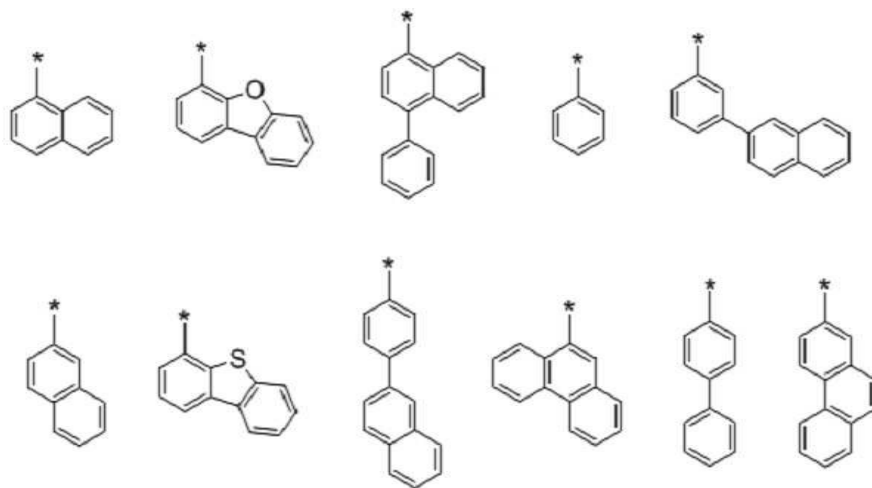
유기 발광 화합물.

청구항 3

제1항에 있어서,

$-L^1-Ar^1$ 및 $-L^2-Ar^2$ 중 적어도 하나는 하기 구조식으로 표시되는 기 중 어느 하나인

유기 발광 화합물.

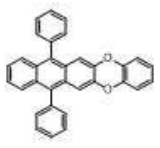
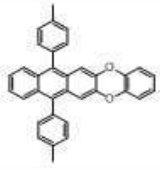
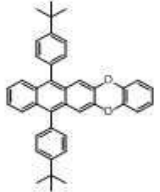
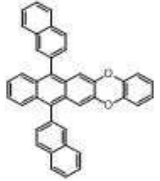
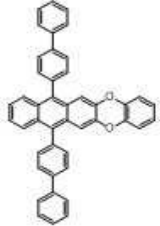
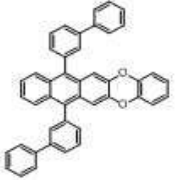
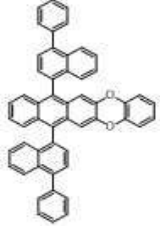
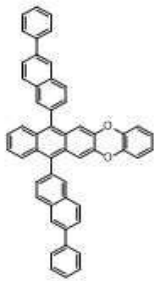
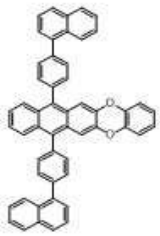


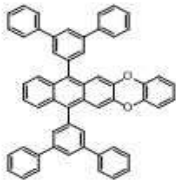
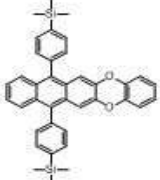
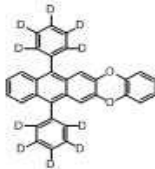
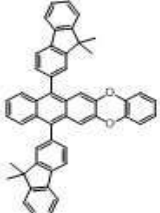
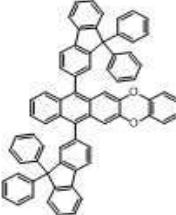
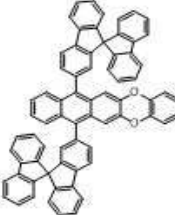
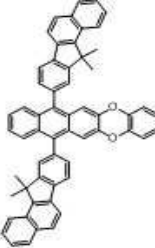
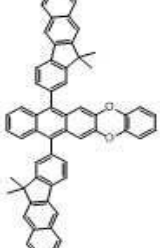
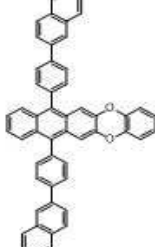
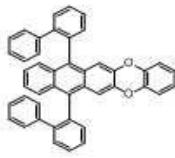
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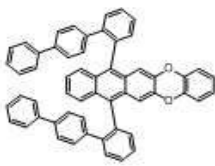
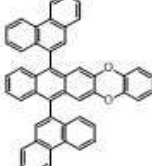
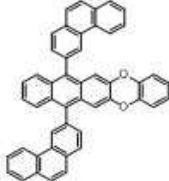
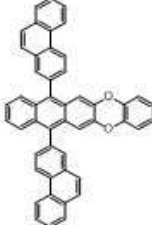
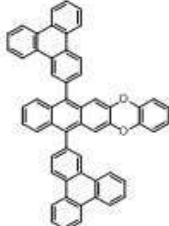
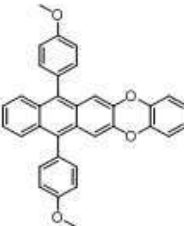
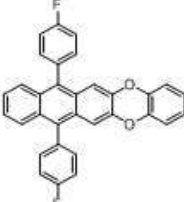
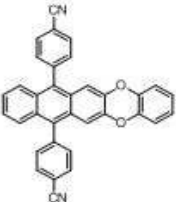
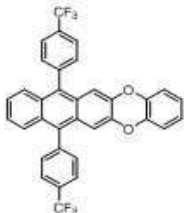
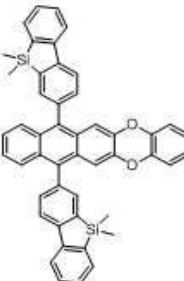
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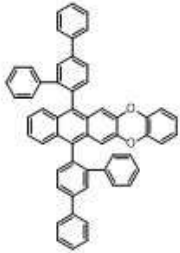
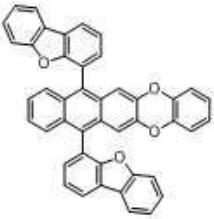
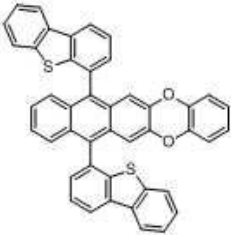
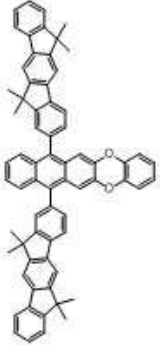
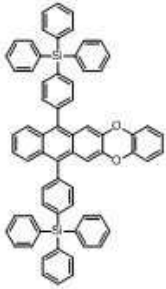
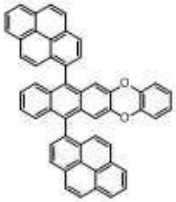
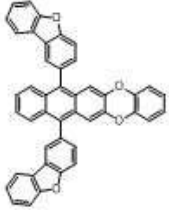
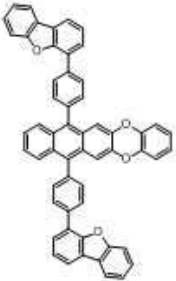
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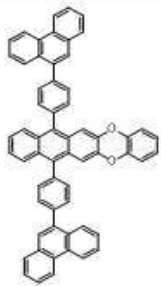
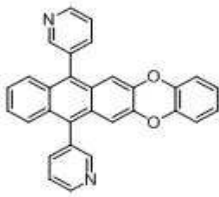
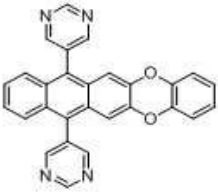
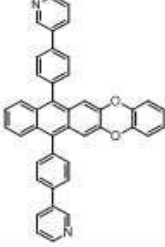
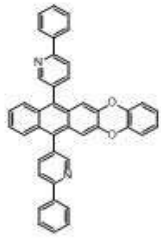
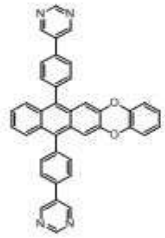
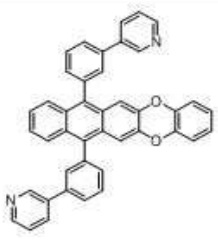
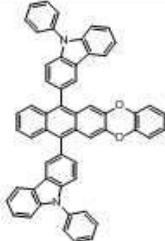
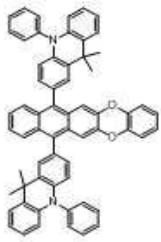
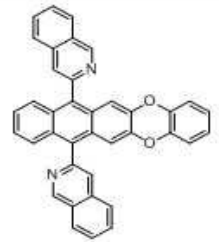
유기 발광 화합물.

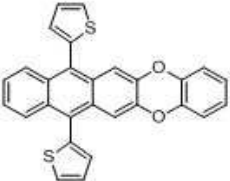
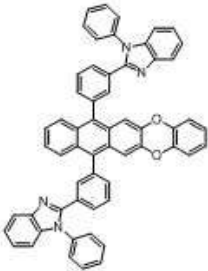
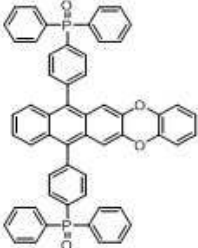
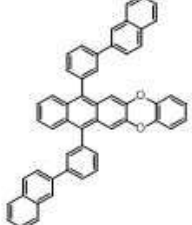
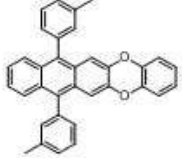
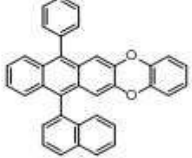
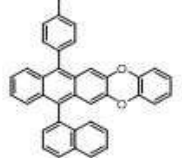
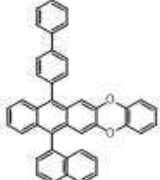
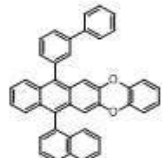
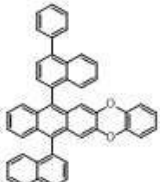
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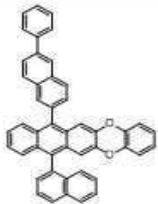
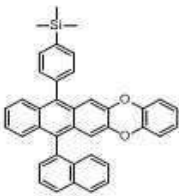
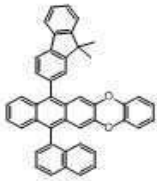
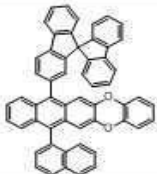
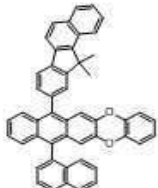
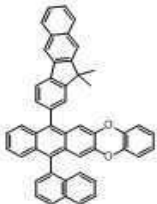
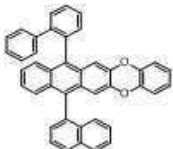
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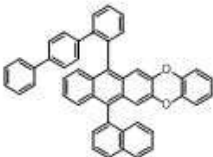
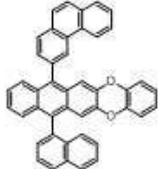
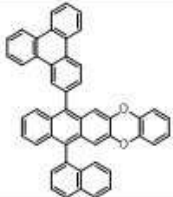
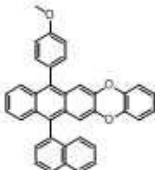
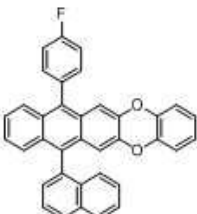
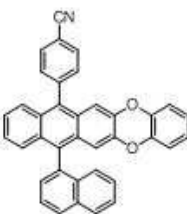
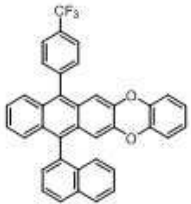
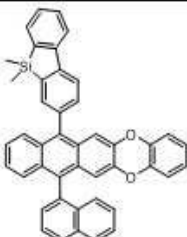
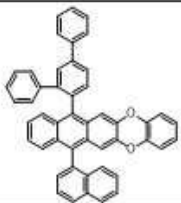
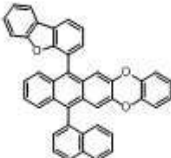
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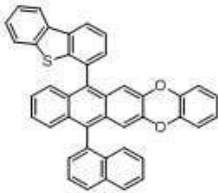
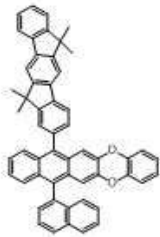
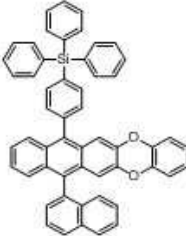
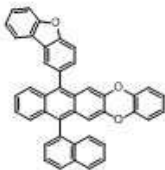
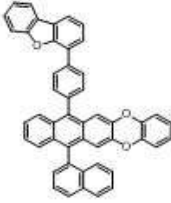
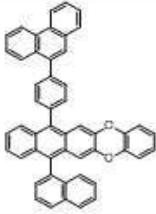
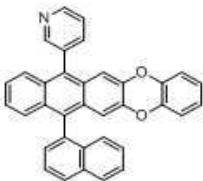
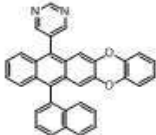
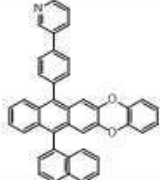
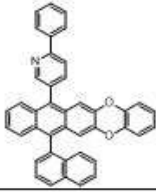
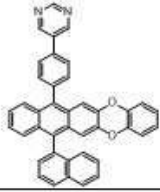
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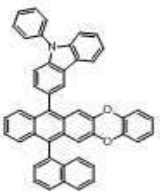
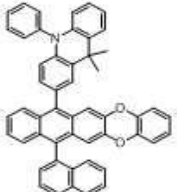
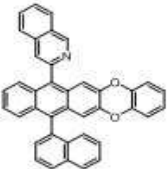
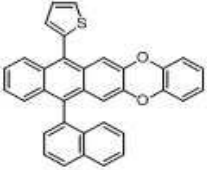
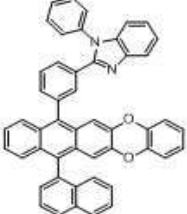
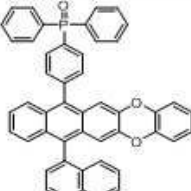
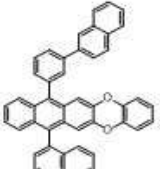
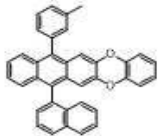
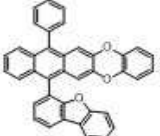
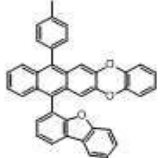
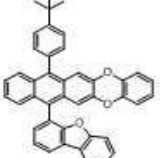
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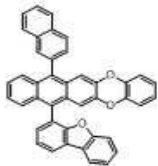
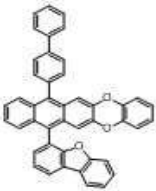
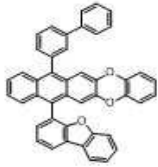
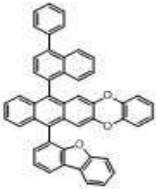
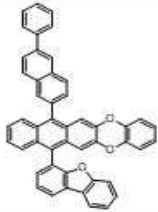
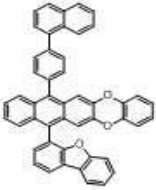
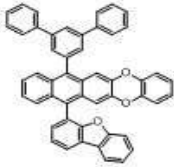
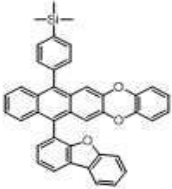
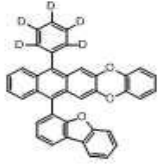
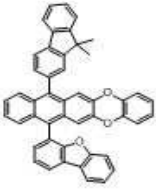
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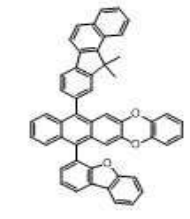
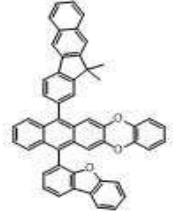
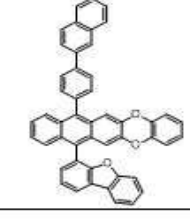
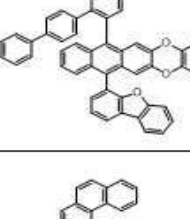
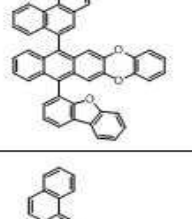
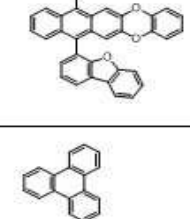
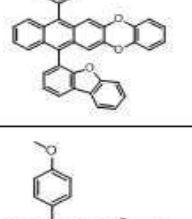
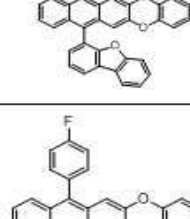
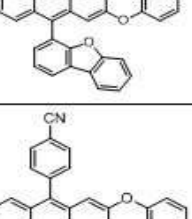
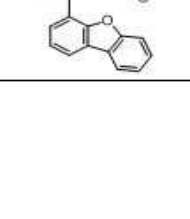
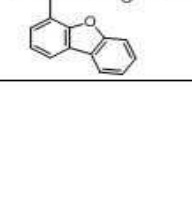
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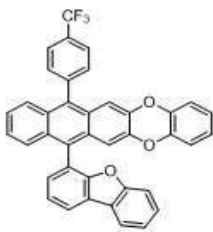
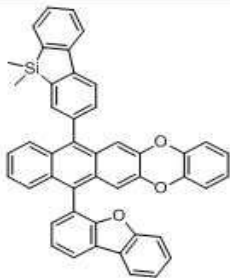
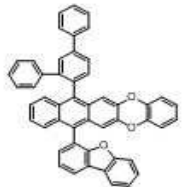
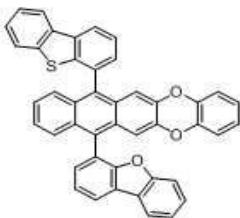
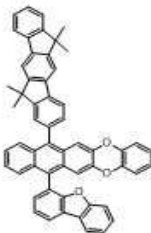
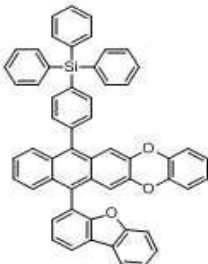
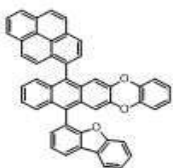
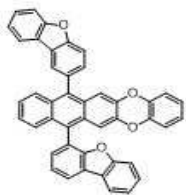
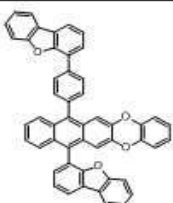
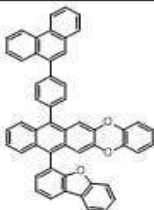
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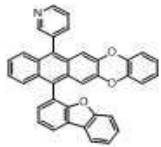
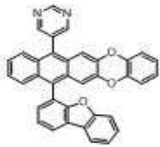
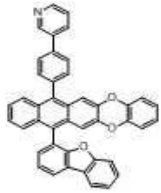
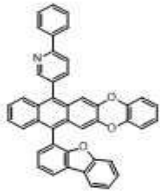
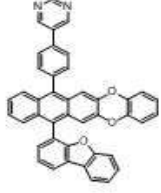
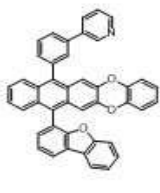
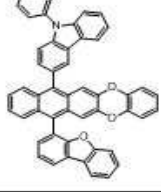
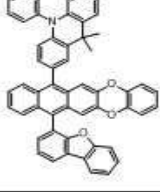
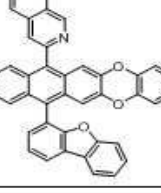
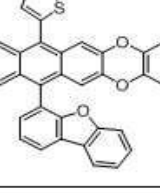
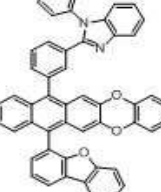
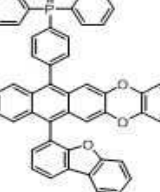
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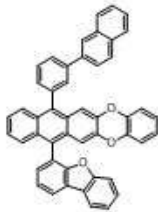
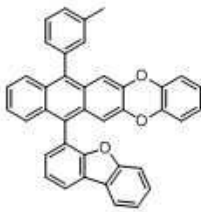
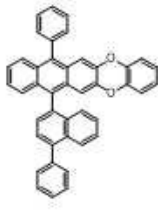
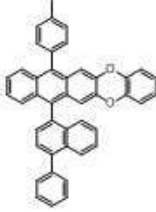
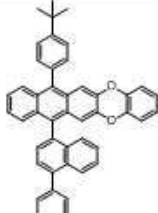
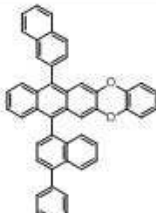
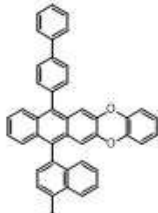
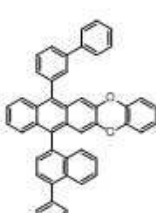
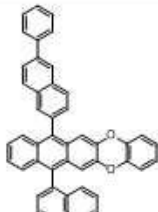
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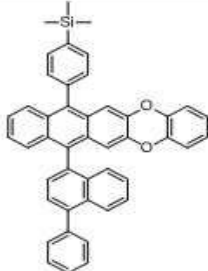
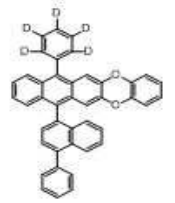
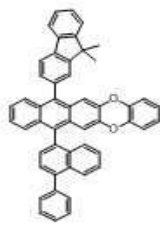
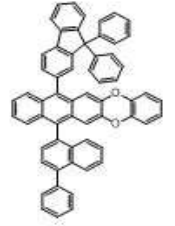
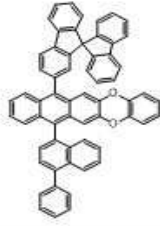
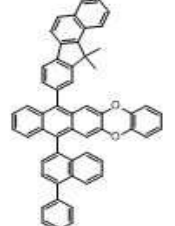
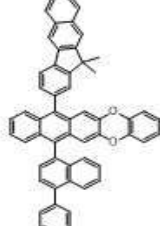
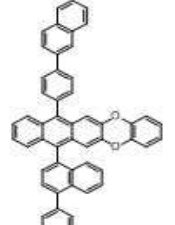
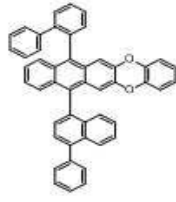
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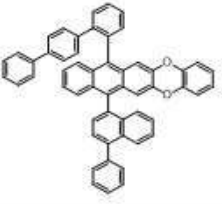
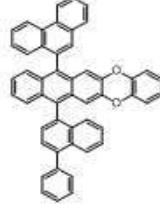
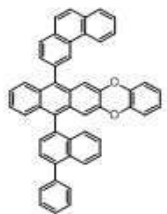
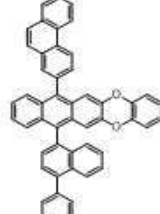
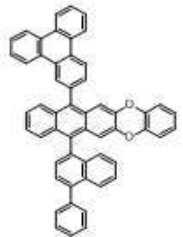
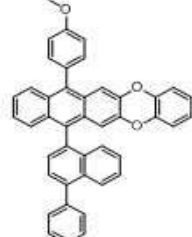
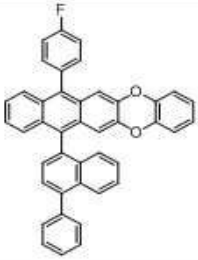
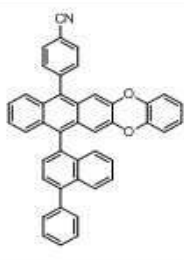
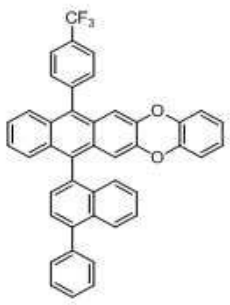
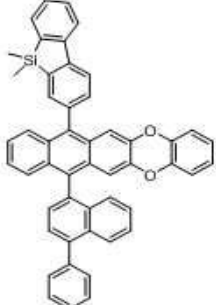
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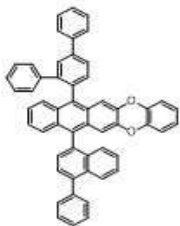
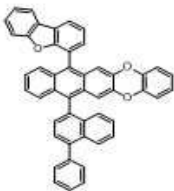
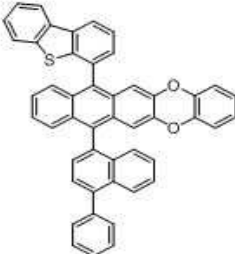
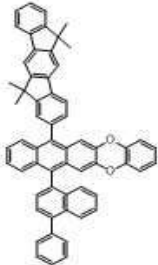
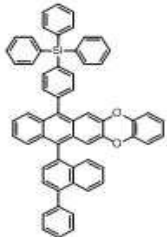
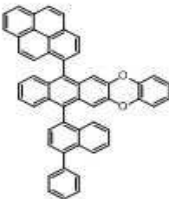
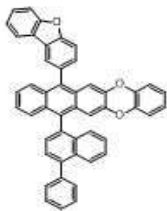
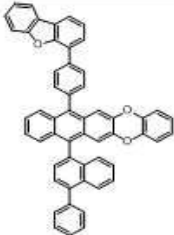
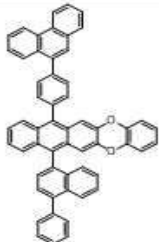
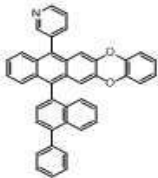
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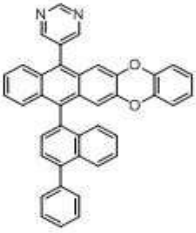
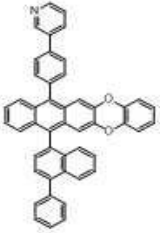
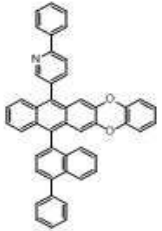
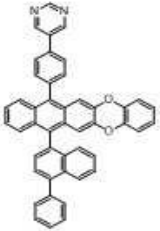
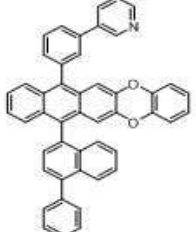
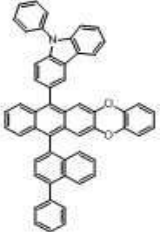
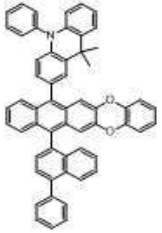
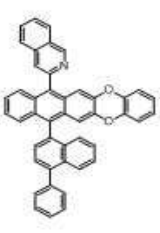
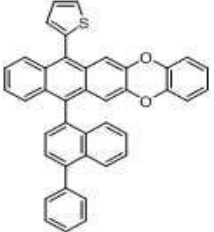
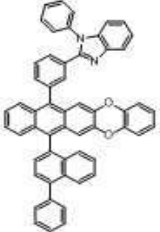
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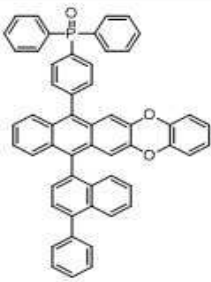
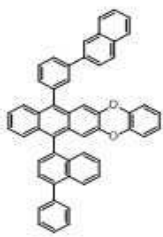
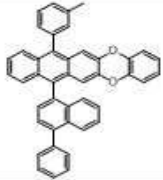
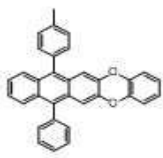
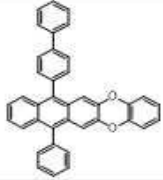
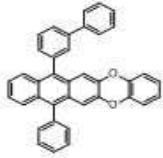
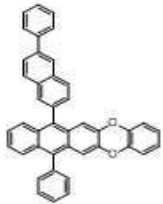
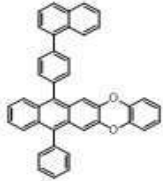
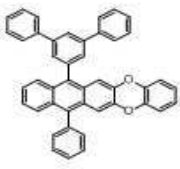
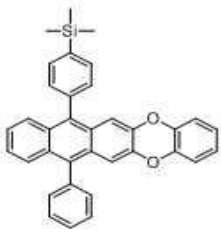
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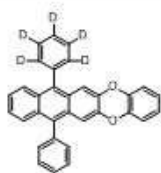
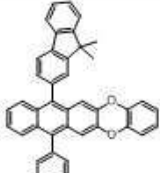
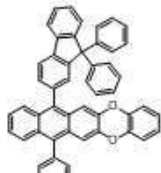
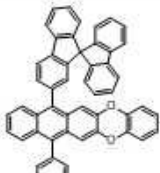
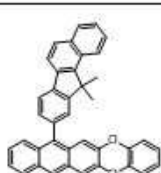
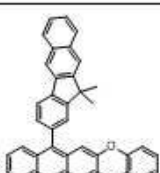
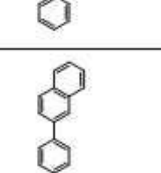
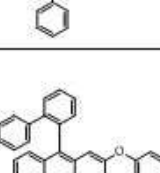
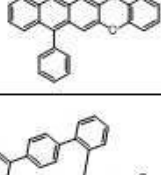
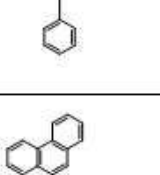
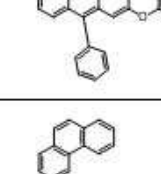
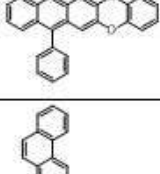
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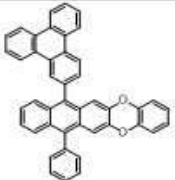
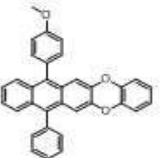
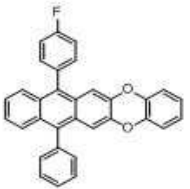
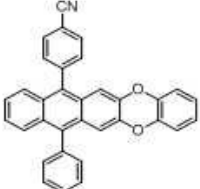
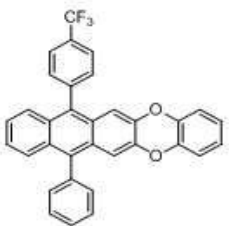
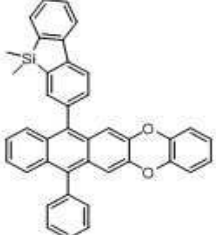
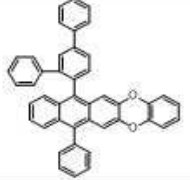
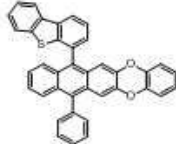
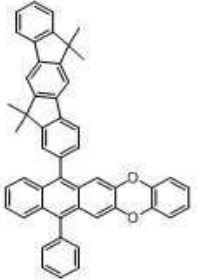
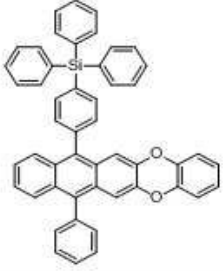
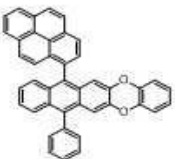
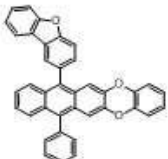
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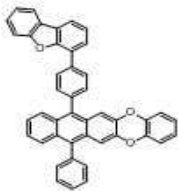
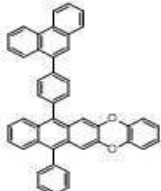
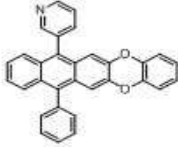
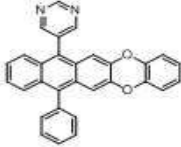
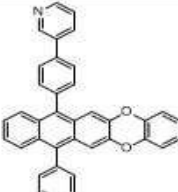
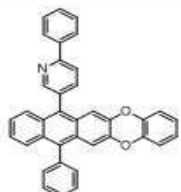
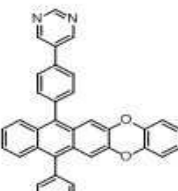
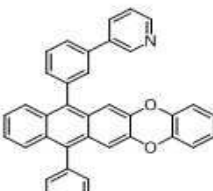
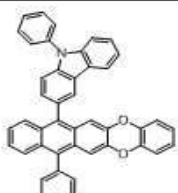
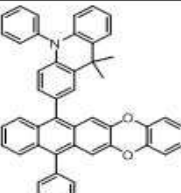
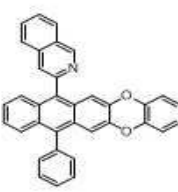
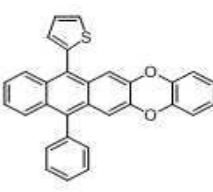
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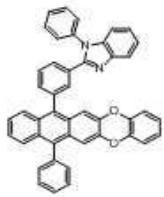
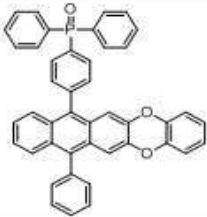
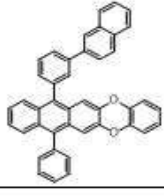
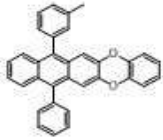
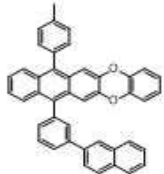
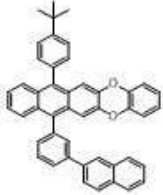
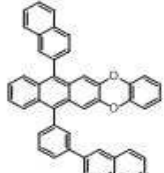
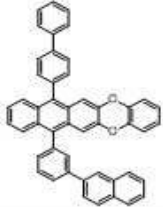
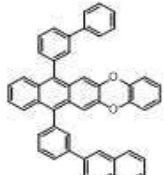
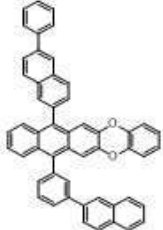
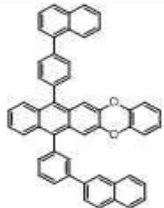
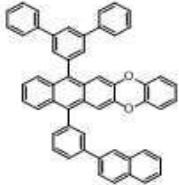
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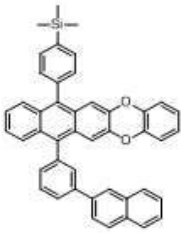
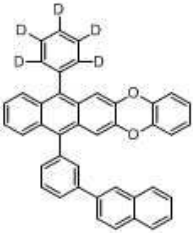
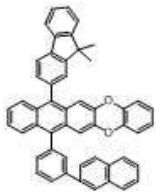
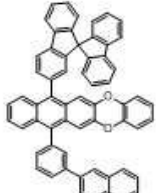
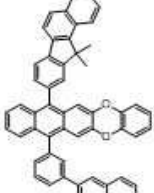
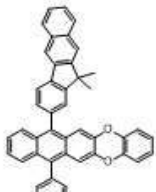
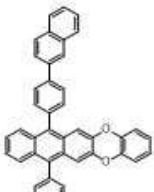
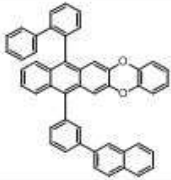
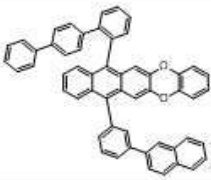
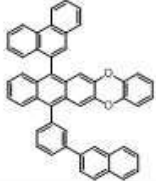
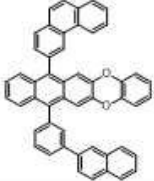
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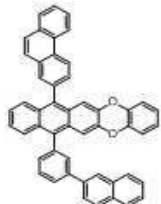
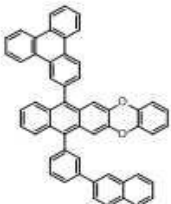
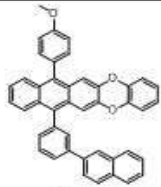
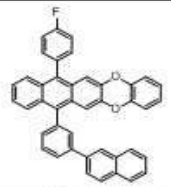
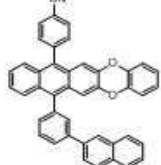
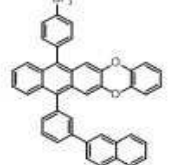
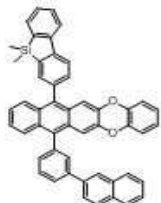
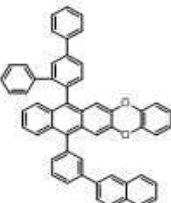
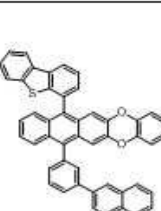
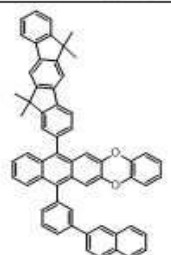
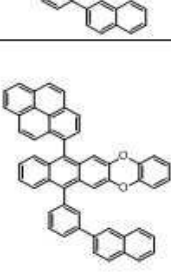
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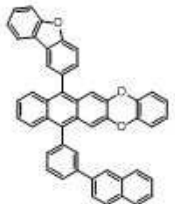
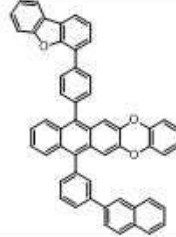
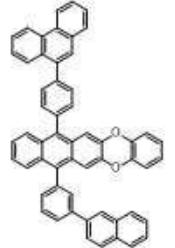
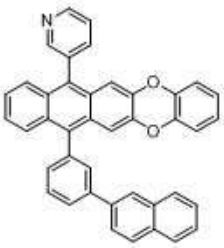
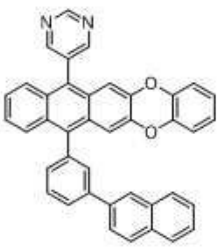
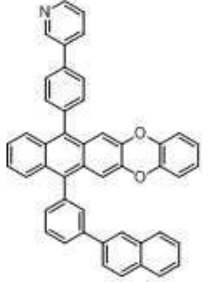
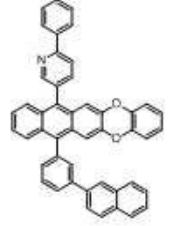
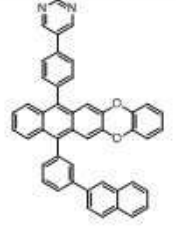
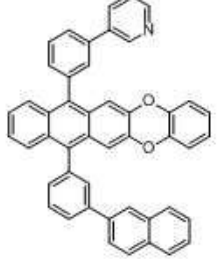
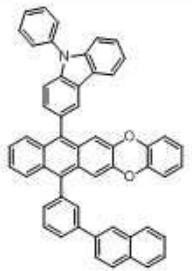
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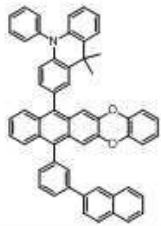
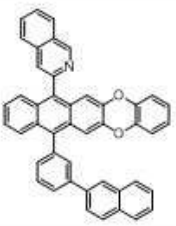
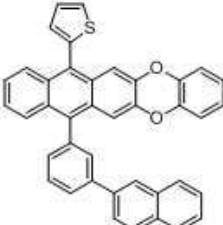
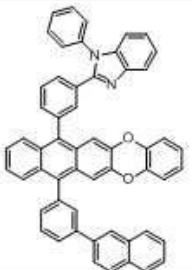
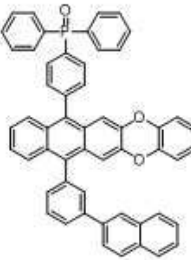
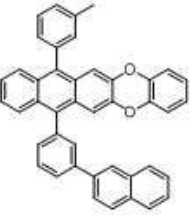
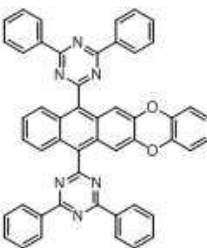
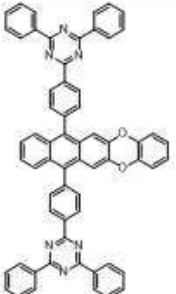
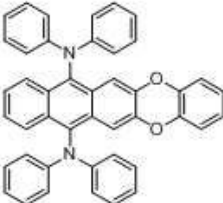
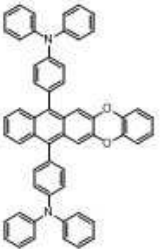
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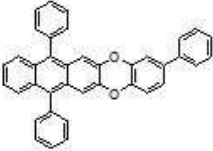
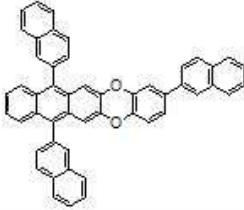
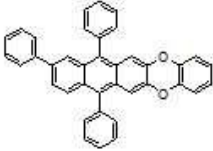
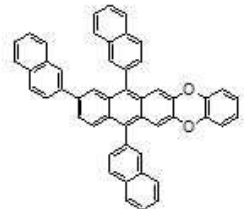
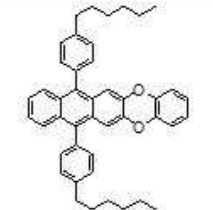
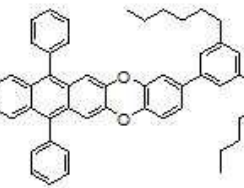
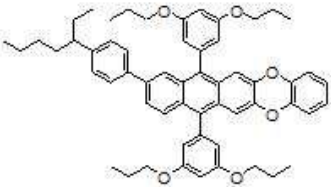
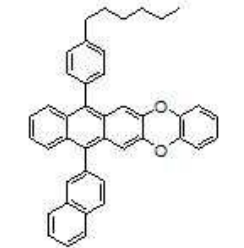
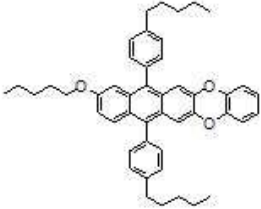
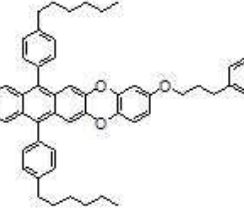
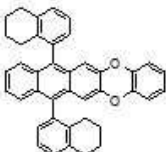
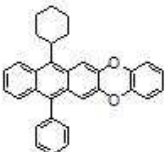
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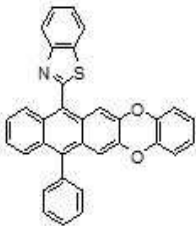
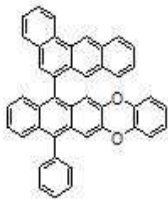
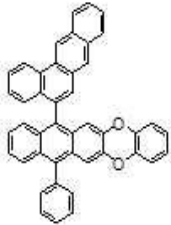
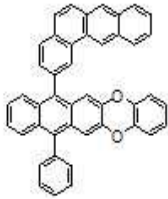
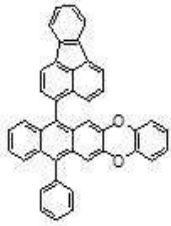
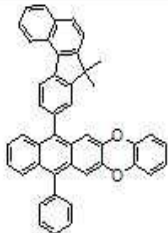
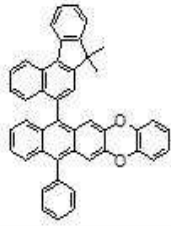
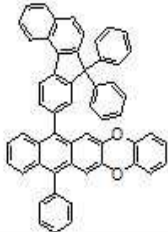
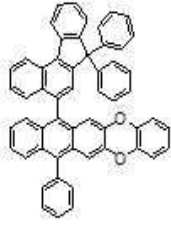
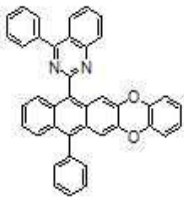
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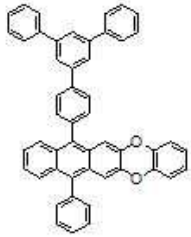
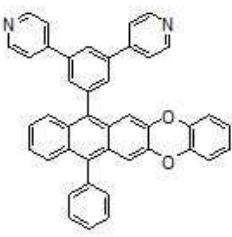
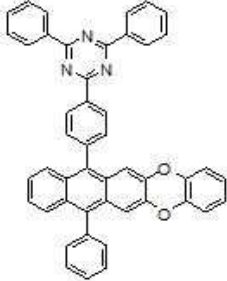
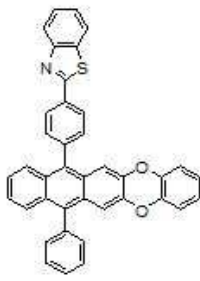
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청구항 5

제1항에 있어서,

상기 유기 발광 화합물이 유기 발광 소자용 유기막의 재료로 사용되는

유기 발광 화합물.

청구항 6

제1항 내지 제5항 중 어느 한 항에 따른 유기 발광 화합물의 적어도 1종 및 인광 또는 형광 도판트를 포함하는 잉크 조성물.

청구항 7

제6항에 있어서,

용매를 더 포함하여 용액 또는 현탁액을 형성한

잉크 조성물.

청구항 8

제6항에 있어서,

안료 또는 염료를 더 포함하는

잉크 조성물.

청구항 9

제6항에 있어서,

인광 도판트 또는 형광 도판트를 더 포함하는

잉크 조성물.

청구항 10

제1 전극, 1층 이상의 유기물층을 포함하는 유기막 및 제2 전극이 적층된 구조를 포함하고, 상기 유기물층은 제1항에 따른 유기 발광 화합물을 적어도 1종 포함하는 유기 발광 소자.

청구항 11

제10항에 있어서,

상기 유기물층이 발광층을 포함하고, 상기 발광층이 제1항에 따른 유기 발광 화합물을 적어도 1종 포함하는 유기 발광 소자.

청구항 12

제11항에 있어서,

상기 유기 발광 화합물은 발광층 중 인광 호스트, 형광 호스트, 인광 도판트, 또는 형광 도판트 재료로서 포함되는

유기 발광 소자.

청구항 13

제10항에 있어서,

상기 유기물층은 정공수송층, 정공주입층, 정공차단층, 전자수송층, 전자주입층 및 전자차단층으로 이루어진 군으로부터 선택된 적어도 하나를 포함하는

유기 발광 소자.

청구항 14

제13항에 있어서,

상기 정공수송층, 상기 정공주입층, 상기 정공차단층, 상기 전자수송층, 상기 전자주입층 또는 상기 전자차단층이 제1항에 따른 유기 발광 화합물을 1종 이상 포함하는

유기 발광 소자.

청구항 15

제10항에 있어서,

상기 유기물층은 제1항에 따른 유기 발광 화합물을 적어도 1종 포함하는 잉크 조성물을 용액 공정에 의해 도포하고 건조시켜 성막하여 제조된

유기 발광 소자.

청구항 16

제10항에 따른 유기 발광 소자를 포함하는 전자 기기.

청구항 17

제16항에 있어서,

상기 전자 기기는: 유기 집적 회로 (O-IC), 유기 전계-효과 트랜지스터 (O-FET), 유기 박막 트랜지스터 (O-TFT), 유기 발광 트랜지스터 (O-LET), 유기 태양 전지 (O-SC), 유기 광학 검출기, 유기 광수용체, 유기 전계-켈치 소자 (O-FQD), 발광 전기화학 전지 (LEC), 유기 레이저 다이오드 (O-레이저) 또는 유기 발광 소자 (OLED)인 전자 기기.

발명의 설명

기술 분야

[0001] 유기 발광 화합물, 잉크 조성물, 이를 포함하는 유기 발광 소자 및 전자 기기에 관한 것이다.

배경 기술

[0002] 전기 발광 소자(electroluminescence device: EL device)는 자체 발광형 표시 소자로서 응답 속도가 빠르고, 시야각이 넓다는 장점을 가지고 있다. 1987년 이스트만 코닥(Eastman Kodak)사는 발광층 재료로서 저분자 방향족 디아민과 알루미늄 착물을 이용한 유기EL 소자를 처음으로 개발하였다[Appl. Phys. Lett. 51, 913, 1987].

[0003] OLED에서 발광 효율을 결정하는 가장 중요한 요인은 발광 재료인데, 발광 재료 중 인광 재료는 이론적으로 형광 재료 대비 4배까지 발광 효율을 개선시킬 수 있다. 현재까지 이리듐(III)착물 계열과 카바졸 계열의 재료들이 인광 발광 재료로 널리 알려져 있으며, 최근 새로운 인광 재료들이 연구되고 있다.

[0004] 유기 전계 발광 현상의 원리는, 음극과 양극 사이에 유기물 층이 있을 때 두 전극 사이에 전압을 걸어주면 음극과 양극으로부터 각각 전자와 정공이 유기물 층으로 주입된다. 유기물 층으로 주입된 전자와 정공은 재결합하여 엑시톤 (exciton)을 형성하고, 이 엑시톤이 다시 바닥 상태로 떨어지면서 빛이 나게 된다. 이러한 원리를 이용하는 유기 발광 소자는 일반적으로 음극과 양극 및 그 사이에 위치한 유기물층, 예컨대 정공주입층, 정공수송층, 발광층, 전자수송층을 포함하는 유기물 층으로 구성될 수 있다.

[0005] 유기 발광 소자에서 사용되는 재료로는 순수 유기물 또는 유기물과 금속이 착물을 이루는 착화합물이 대부분을 차지하고 있으며, 용도에 따라 정공주입 재료, 정공수송 재료, 발광 재료, 전자수송 재료, 전자주입 재료 등으로 구분될 수 있다. 여기서, 정공주입 재료나 정공수송 재료로는 p-타입의 성질을 가지는 유기 재료, 즉 쉽게 산화가 되고 산화시에 전기화학적으로 안정한 상태를 가지는 유기물이 주로 사용되고 있다. 한편, 전자주입 재료나 전자수송 재료로는 n-타입 성질을 가지는 유기 재료, 즉 쉽게 환원이 되고 환원시에 전기화학적으로 안정한 상태를 가지는 유기물이 주로 사용되고 있다. 발광층 재료로는 p-타입 성질과 n-타입 성질을 동시에 가진 재료, 즉 산화와 환원 상태에서 모두 안정한 형태를 갖는 재료가 바람직하며, 엑시톤이 형성되었을 때 이를 빛으로 전환하는 발광 효율이 높은 재료가 바람직하다. 따라서, 당 기술 분야에서는 상기와 같은 요건을 갖춘 새로운 유기 재료의 개발이 요구되고 있다.

발명의 내용

해결하려는 과제

[0006] 본 발명의 일 구현예는 적절한 에너지 준위, 전기화학적 안정성 및 열적 안정성을 가지는 신규한 유기 발광 화합물을 제공한다.

[0007] 본 발명의 다른 구현예는 상기 유기 발광 화합물을 포함하는 잉크 조성물을 제공한다.

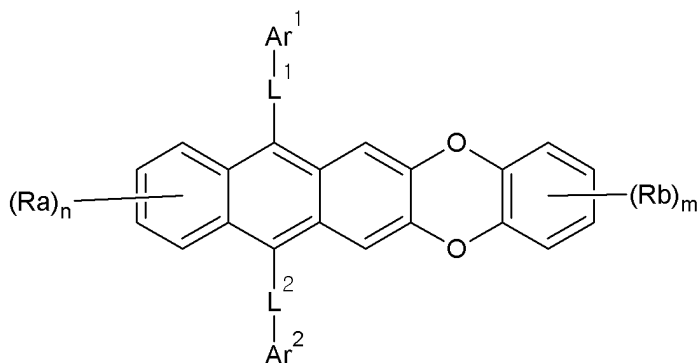
[0008] 본 발명의 또 다른 구현예는 상기 유기 발광 화합물을 포함하는 유기 발광 소자를 제공한다.

[0009] 본 발명의 또 다른 구현에는 상기 유기 발광 소자를 적용한 전자 기기를 제공한다.

과제의 해결 수단

[0010] 본 발명의 일 구현예에서, 하기 화학식 1로 표시되는 유기 발광 화합물을 제공한다.

[0011] <화학식 1>



[0012]

[0013] 상기 식에서,

[0014] Ar¹ 및 Ar²는, 각각 독립적으로, 치환 또는 비치환된 C6-C60의 아릴기, 치환 또는 비치환된 C3-C60의 헤테로아릴기, 치환 또는 비치환된 C3-C60의 시클로알킬기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬기, -N(R1)(R2), -P(O)(R3)(R4) 또는 -Si(R5)(R6)(R7)이고, 상기 R1, R2, R3, R4, R5, R6 및 R7은, 각각 독립적으로, C6-C50의 아릴기 또는 C3-C50의 헤테로아릴기이고,

[0015] 상기 Ar¹ 및 Ar²이 치환된 경우의 치환기는 중수소, 불소, C1-C30의 알킬기, C6-C30의 아릴기, C2-C30의 헤테로아릴기, C1-C30의 알콕시기, C1-C30의 플루오로알킬기, -Si(CH₃)₃ 및 -CN로 이루어진 군에서 선택된 하나이고;

[0016] L¹ 및 L²는, 각각 독립적으로, 단일 결합, 치환 또는 비치환된 C6-C60의 아릴렌기, 치환 또는 비치환된 C3-C60의 헤테로아릴렌기, 치환 또는 비치환된 C3-C60의 시클로알킬렌기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬렌기 및 이들의 조합으로 이루어진 군으로부터 선택된 하나이고,

[0017] 상기 L¹ 및 L²이 치환된 경우의 치환기는 C1-C20의 알킬기 및 C3-C20의 아릴기로 이루어진 군에서 선택된 적어도 하나이고;

[0018] Ra 및 Rb는, 각각 독립적으로, 치환 또는 비치환된 C6-C60의 아릴기, 치환 또는 비치환된 C3-C60의 헤테로아릴기, 치환 또는 비치환된 C3-C60의 시클로알킬기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬기, -N(R1)(R2), -P(O)(R3)(R4) 또는 -Si(R5)(R6)(R7)이고, 상기 R1, R2, R3, R4, R5, R6 및 R7은, 각각 독립적으로, C6-C50의 아릴기 또는 C3-C50의 헤테로아릴기이고,

[0019] 상기 Ra 및 Rb가 치환된 경우의 치환기는 C1-C30의 알킬기 또는 C1-C30의 알콕시기이고;

[0020] n 및 m은, 각각 독립적으로, 0 내지 4의 정수이다.

[0021] 본 발명의 다른 구현예에서, 상기 유기 발광 화합물의 적어도 1종을 포함하는 잉크 조성물을 제공한다.

[0022] 본 발명의 또 다른 구현예에서, 제1 전극, 1층 이상의 유기물층 및 제2 전극이 적층된 구조를 포함하고, 상기 유기물층은 상기 유기 발광 화합물을 적어도 1종 포함하는 유기 발광 소자를 제공한다.

[0023] 본 발명의 또 다른 구현예에서, 상기 유기 발광 소자를 포함하는 전자 기기를 제공한다.

발명의 효과

[0024] 상기 유기 발광 화합물은 유기 발광 소자에서 사용 가능한 물질에 요구되는 조건, 예컨대 적절한 에너지 준위,

전기화학적 안정성 및 열적 안정성 등을 모두 우수하게 만족시킬 수 있으며, 치환기에 따라 유기 발광 소자에서 요구되는 다양한 역할을 할 수 있다.

도면의 간단한 설명

[0025]

도 1은 실시예에서 제조된 화합물 [5]의 $^1\text{H-NMR}$ 측정 결과이다.

도 2는 실시예에서 제조된 화합물 [5]에 대한 열중량분석 (thermogravimetric analysis, TGA) 그래프이다.

도 3은 실시예에서 제조된 화합물 [5]에 대한 시차주사열량 (differential scanning calorimetry, DSC) 측정 그래프이다.

도 4는 실시예에서 제조된 화합물 [5]에 대한 UV 흡수스펙트럼이다.

도 5는 실시예에서 제조된 화합물 [5]에 대한 광발광 (Photoluminescence, PL) 측정 그래프 이다.

발명을 실시하기 위한 구체적인 내용

[0026]

이하, 본 발명의 구현예를 상세히 설명하기로 한다. 다만, 이는 예시로서 제시되는 것으로, 이에 의해 본 발명이 제한되지는 않으며 본 발명은 후술할 청구항의 범주에 의해 정의될 뿐이다.

[0027]

본 명세서에서 "치환"된 경우는 별도의 정의가 없는 한, C1-C50의 알킬기, C3-C50의 시클로알킬기, C2-C50의 알케닐기, C3-C50의 시클로알케닐기, C2-C50의 알키닐기, C5-C50의 시클로알키닐기, 시아노기, C1-C20의 알콕시기, C6-C60의 아릴기 및 C7-C60의 아릴알킬기 및 이들의 조합으로 이루어진 군에서 선택된 치환기로 치환된 경우를 포함한다.

[0028]

본 명세서에서 "이들의 조합"이란 별도의 정의가 없는 한, 둘 이상의 치환기가 연결기로 결합되어 있거나, 둘 이상의 치환기가 축합하여 결합되어 있는 것을 의미한다.

[0029]

또한, 본 명세서에서 "*"는 동일하거나 상이한 원자 또는 화학식과 연결되는 부분을 의미한다.

[0030]

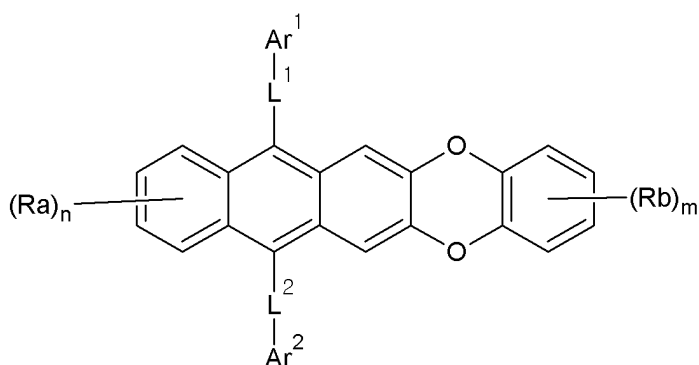
본 명세서에서 "헤테로"란 별도의 정의가 없는 한, 하나의 화합물 또는 치환기 내에 헤테로 원자를 포함함을 의미하고, 상기 헤테로 원자는 N, O, S, P 및 이들의 조합으로 이루어진 군에서 선택된 하나일 수 있다. 예를 들어, 상기 하나의 화합물 또는 치환기 내에 헤테로 원자를 1 내지 3 포함하고, 나머지는 탄소인 경우를 의미할 수 있다.

[0031]

본 발명의 일 구현예에서, 신규한 하기 화학식 1로 표시되는 유기 발광 화합물을 제공한다.

[0032]

<화학식 1>



[0033]

상기 식에서,

[0035]

Ar^1 및 Ar^2 는, 각각 독립적으로, 치환 또는 비치환된 C6-C60의 아릴기, 치환 또는 비치환된 C3-C60의 헤테로아릴기, 치환 또는 비치환된 C3-C60의 시클로알킬기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬기, $-\text{N}(\text{R}1)(\text{R}2)$, $-\text{P}(\text{O})(\text{R}3)(\text{R}4)$ 또는 $-\text{Si}(\text{R}5)(\text{R}6)(\text{R}7)$ 이고, 상기 R1, R2, R3, R4, R5, R6 및 R7은, 각각 독립적으

로, C6-C50의 아릴기 또는 C3-C50의 헤테로아릴기이고,

[0036] 상기 Ar^1 및 Ar^2 이 치환된 경우의 치환기는 중수소, 불소, C1-C30의 알킬기, C6-C30의 아릴기, C2-C30의 헤테로아릴기, C1-C30의 알콕시기, C1-C30의 플루오로알킬기, $-Si(CH_3)_3$ 및 $-CN$ 로 이루어진 군에서 선택된 하나이고;

[0037] L^1 및 L^2 는, 각각 독립적으로, 단일 결합, 치환 또는 비치환된 C6-C60의 아릴렌기, 치환 또는 비치환된 C3-C60의 헤테로아릴렌기, 치환 또는 비치환된 C3-C60의 시클로알킬렌기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬렌기 및 이들의 조합으로 이루어진 군으로부터 선택된 하나이고,

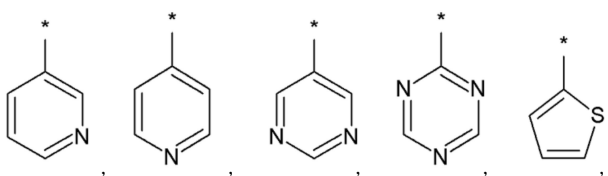
[0038] 상기 L^1 및 L^2 이 치환된 경우의 치환기는 C1-C20의 알킬기 및 C3-C20의 아릴기로 이루어진 군에서 선택된 적어도 하나이고;

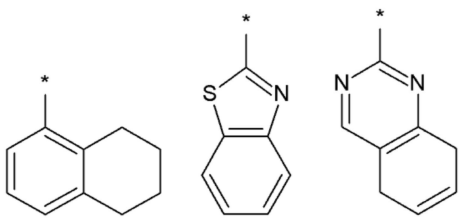
[0039] Ra 및 Rb는, 각각 독립적으로, 치환 또는 비치환된 C6-C60의 아릴기, 치환 또는 비치환된 C3-C60의 헤테로아릴기, 치환 또는 비치환된 C3-C60의 시클로알킬기, 치환 또는 비치환된 C2-C60의 헤테로시클로알킬기, $-N(R1)(R2)$, $-P(O)(R3)(R4)$ 또는 $-Si(R5)(R6)(R7)$ 이고, 상기 R1, R2, R3, R4, R5, R6 및 R7은, 각각 독립적으로, C6-C50의 아릴기 또는 C3-C50의 헤테로아릴기이고,

[0040] 상기 Ra 및 Rb가 치환된 경우의 치환기는 C1-C30의 알킬기 또는 C1-C30의 알콕시기이고;

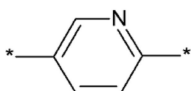
[0041] n 및 m은, 각각 독립적으로, 0 내지 4의 정수이다.

[0042] 상기 유기 발광 화합물은, 구체적으로,

[0043] Ar^1 및 Ar^2 는, 각각 독립적으로, 페닐기, 시클로헥산기, ,

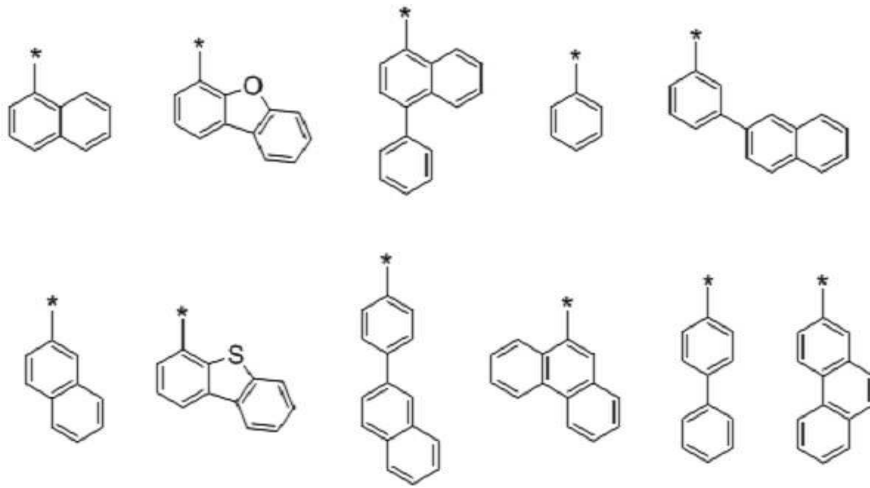
, 3원 내지 6원환의 고리가 2 내지 5개 융합되거나, 축합되거나 또는 스피로 구조로 연결된 C6-C60의 고리기 및 이들의 조합으로 이루어진 군으로부터 선택된 하나이고, 상기 3원 내지 6원환의 고리는 지환족 또는 방향족고리일 수 있으며 헤테로원자를 포함하거나 포함하지 않을 수 있고,

[0044] 상기 정의된 Ar^1 및 Ar^2 중 수소 원자는 C1-C30 알킬기 또는 C6-C30 아릴기로 치환 또는 비치환되고;

[0045] L^1 및 L^2 는, 각각 독립적으로, 단일 결합, 비페닐렌, C1-C20 알킬기 또는 332]로 치환 또는 비치환된 페닐렌기, , 또는 3원 내지 6원환의 고리가 2 내지 5개 융합되거나, 축합되거나 또는 스피로 구조로 연결된 C6-C60의 2가 고리기이고, 상기 3원 내지 6원환의 고리는 지환족 또는 방향족 고리일 수 있으며 헤테로원자를 포함하거나 포함하지 않을 수 있고,

[0046] 상기 정의된 L^1 및 L^2 중 수소 원자는 페닐기로 치환 또는 비치환될 수 있다.

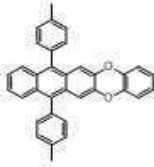
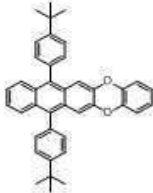
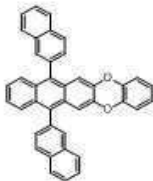
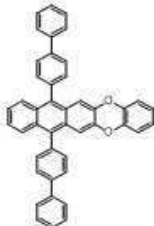
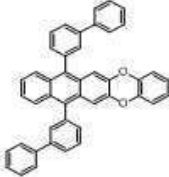
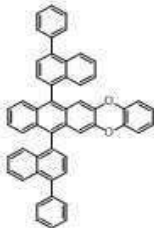
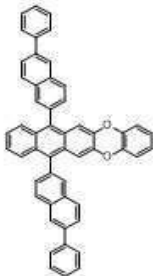
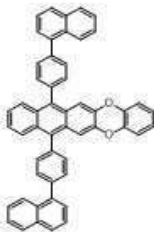
[0047] 일 구현예에서, 상기 화학식 1에서, $-L^1-Ar^1$ 및 $-L^2-Ar^2$ 중 적어도 하나는 하기 구조식으로 표시되는 기 중 어느 하나일 수 있다.



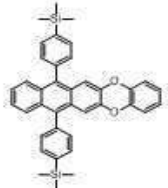
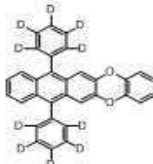
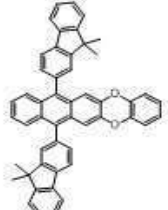
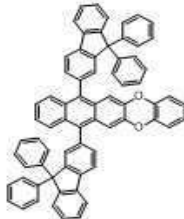
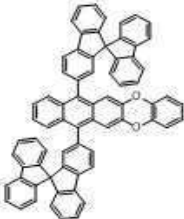
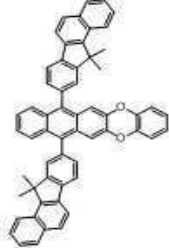
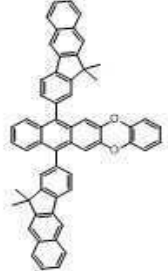
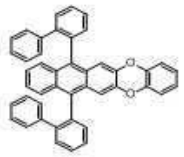
[0048]

[0049] 예를 들어, 상기 유기 발광 화합물은 하기 표 1에 기재된 1 내지 334 중의 어느 하나의 화합물일 수 있다.

표 1

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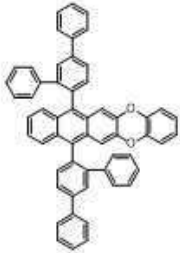
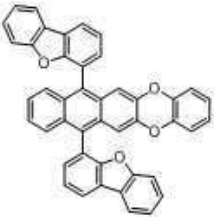
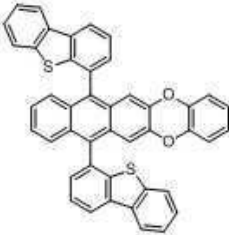
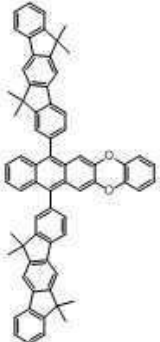
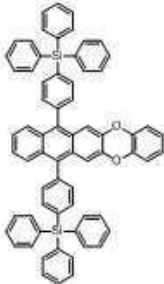
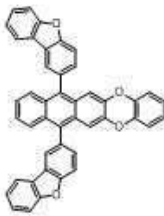
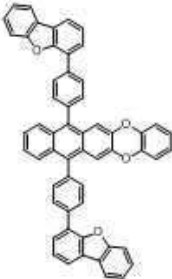
[0050]

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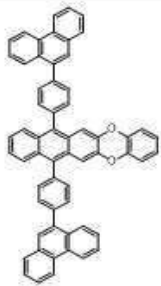
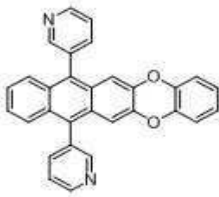
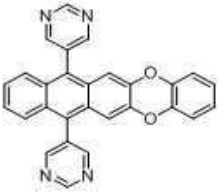
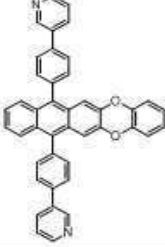
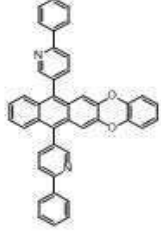
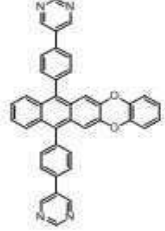
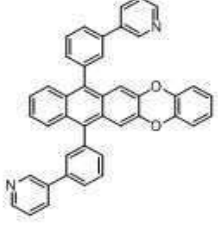
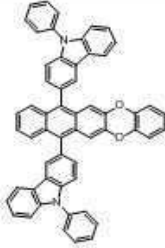
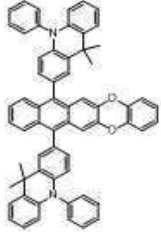
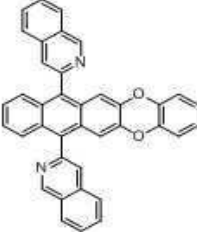
[0051]

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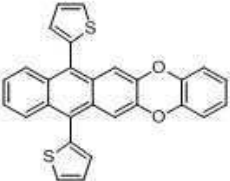
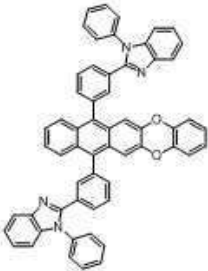
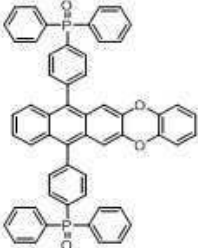
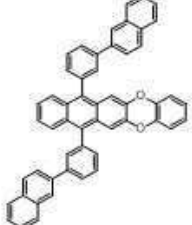
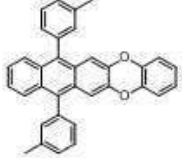
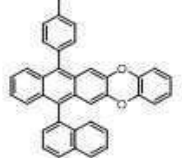
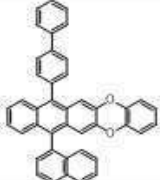
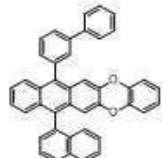
[0052]

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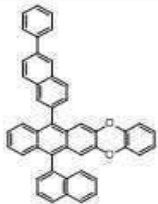
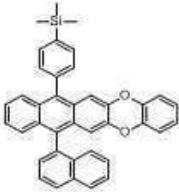
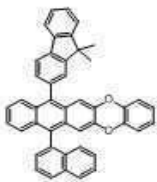
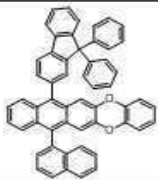
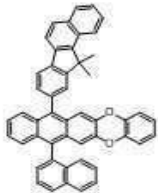
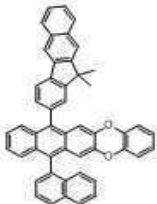
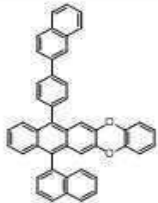
[0053]

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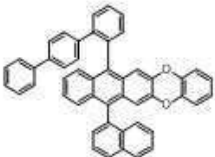
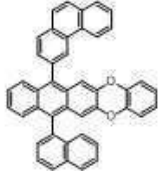
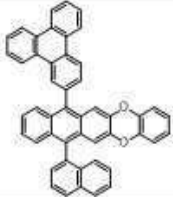
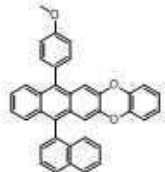
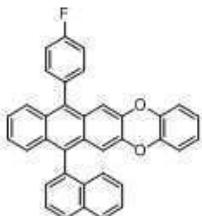
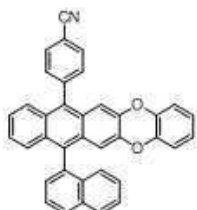
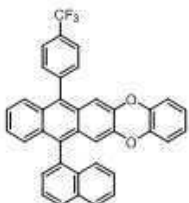
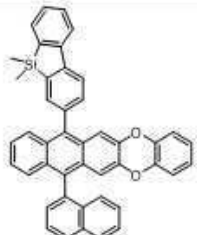
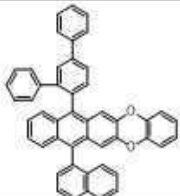
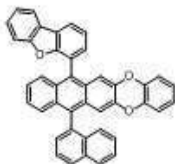
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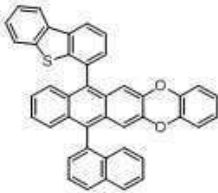
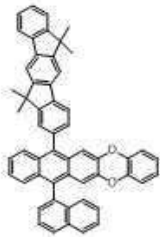
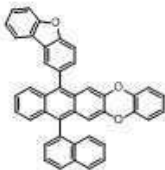
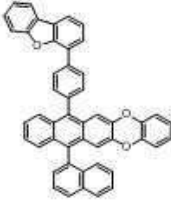
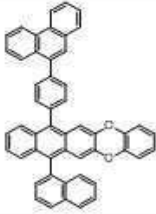
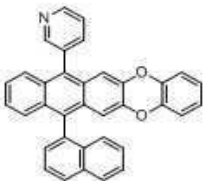
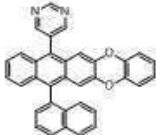
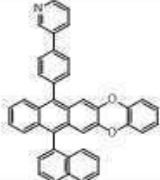
[0055]

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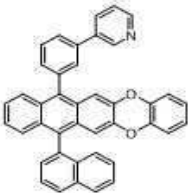
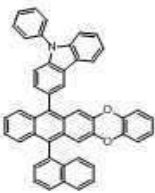
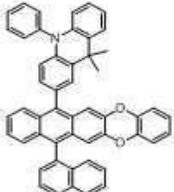
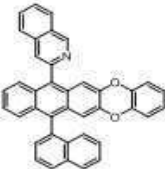
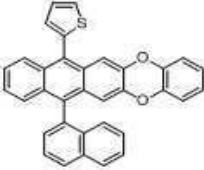
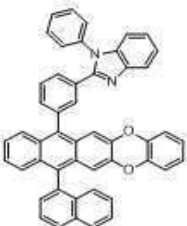
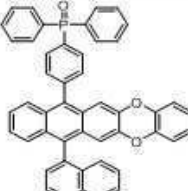
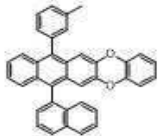
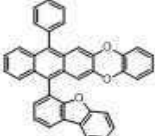
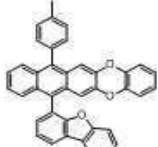
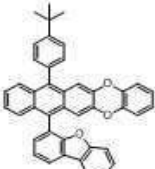
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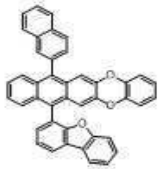
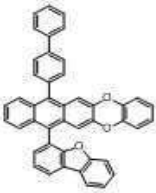
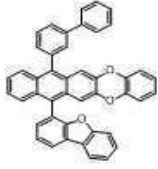
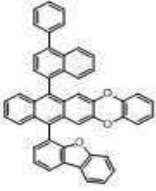
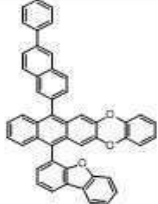
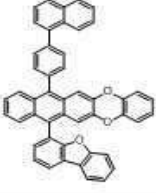
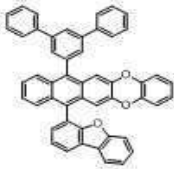
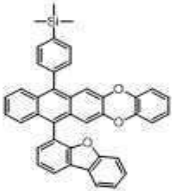
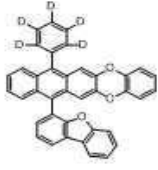
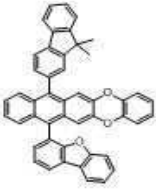
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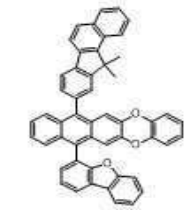
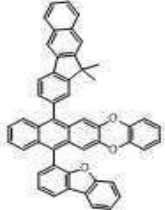
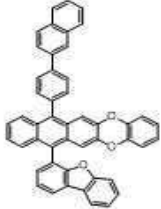
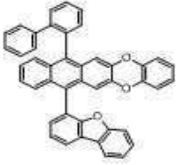
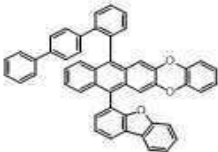
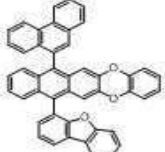
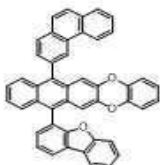
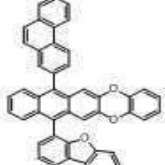
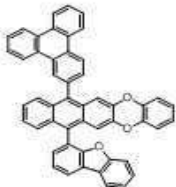
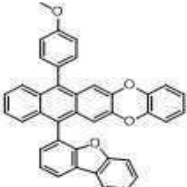
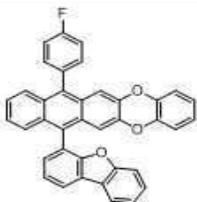
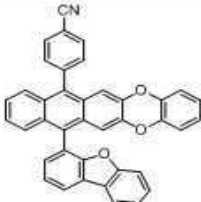
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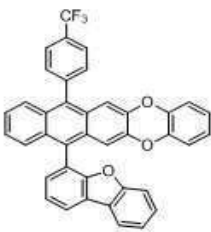
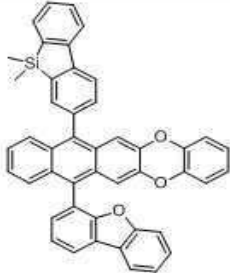
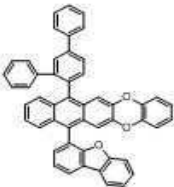
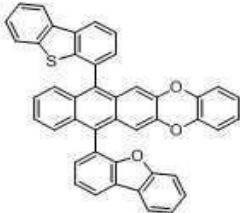
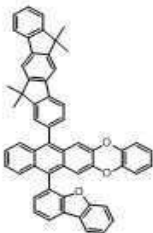
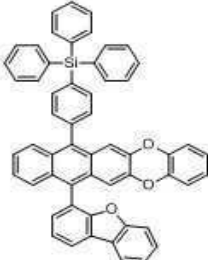
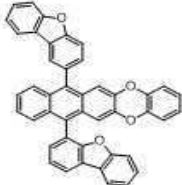
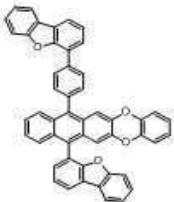
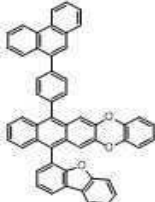
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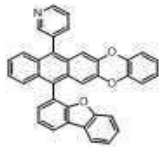
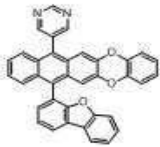
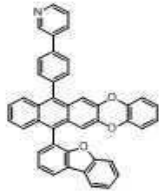
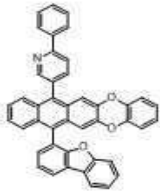
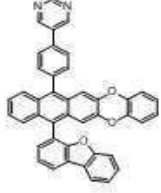
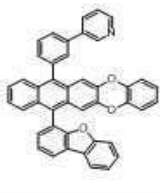
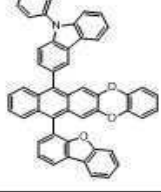
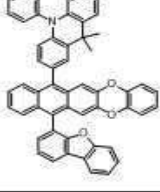
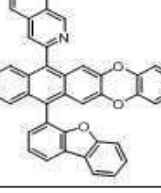
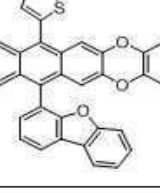
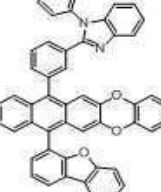
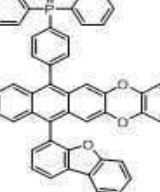
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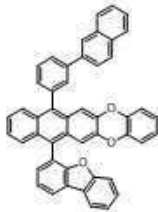
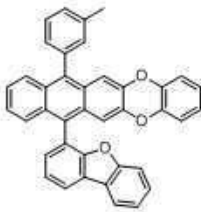
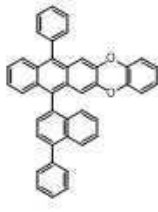
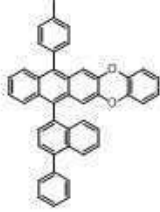
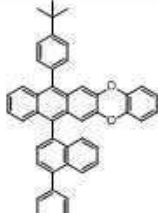
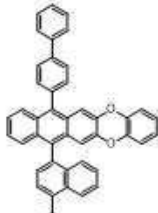
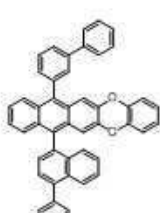
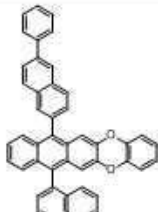
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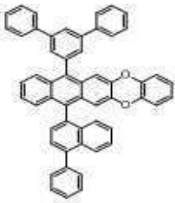
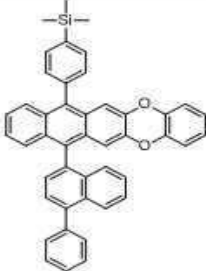
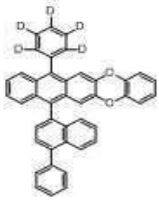
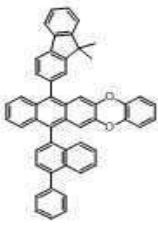
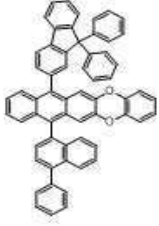
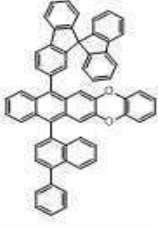
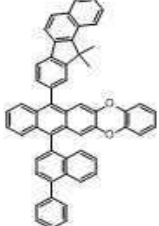
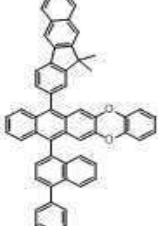
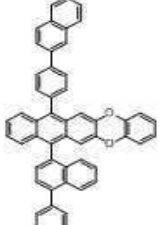
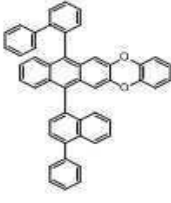
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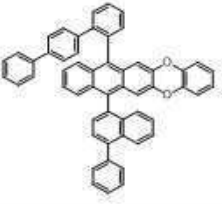
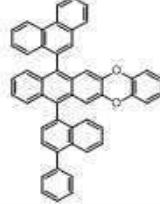
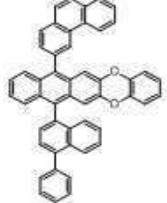
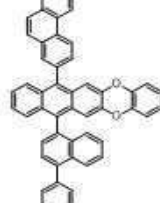
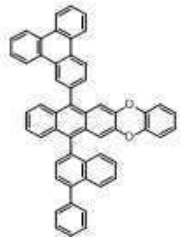
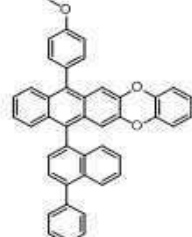
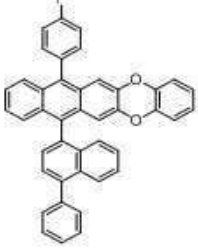
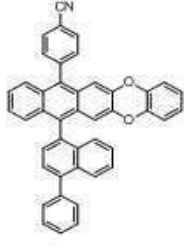
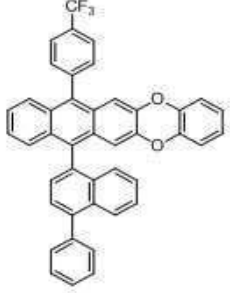
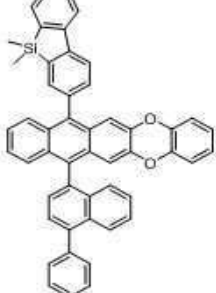
[0063]

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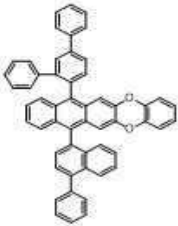
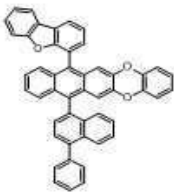
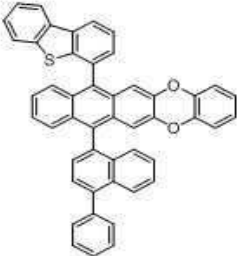
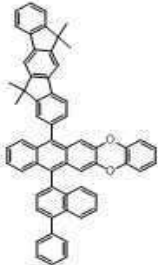
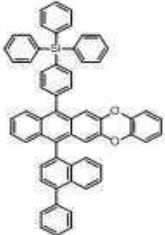
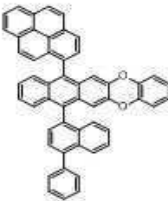
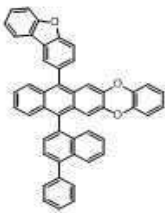
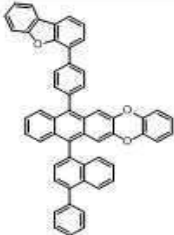
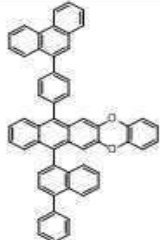
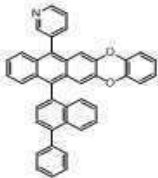
[0064]

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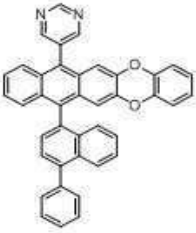
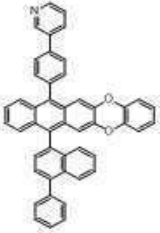
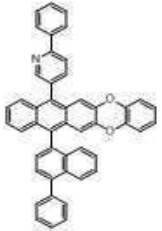
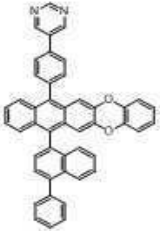
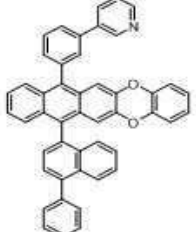
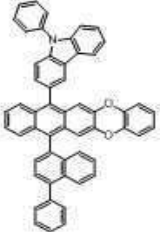
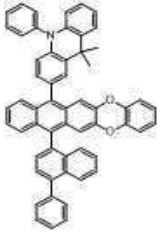
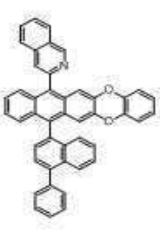
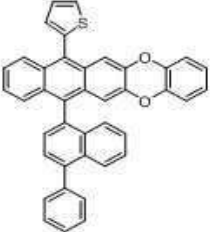
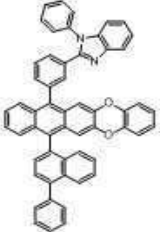
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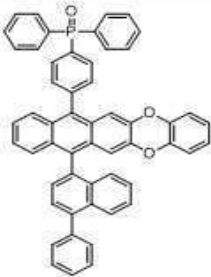
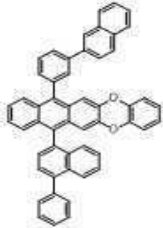
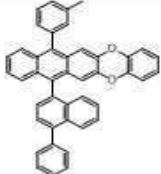
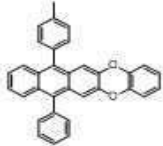
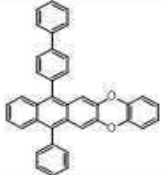
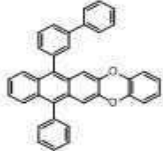
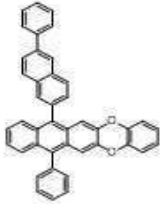
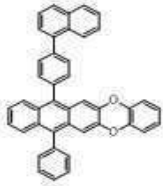
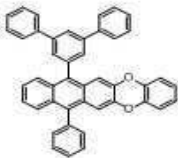
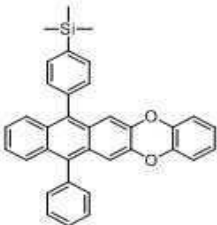
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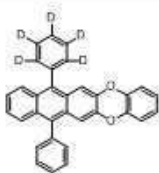
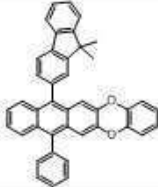
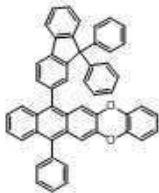
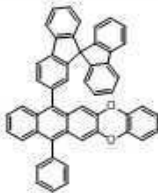
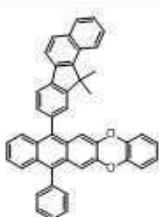
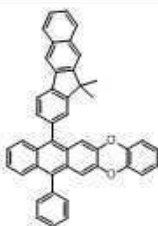
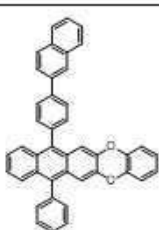
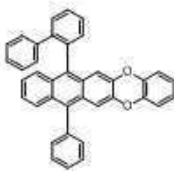
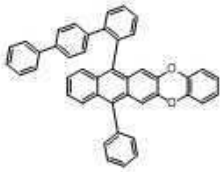
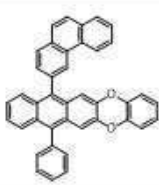
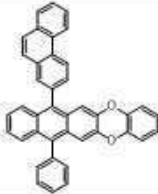
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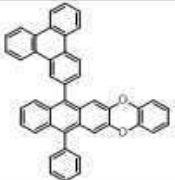
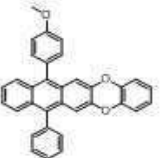
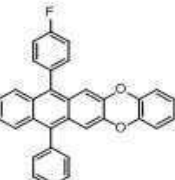
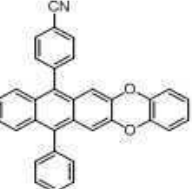
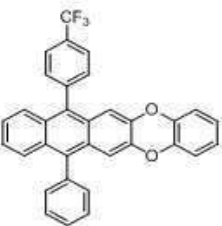
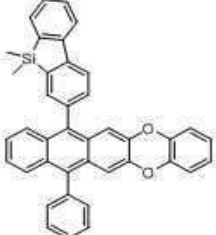
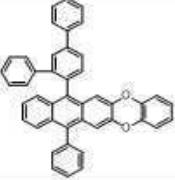
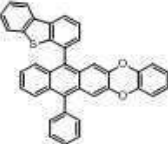
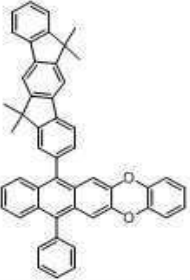
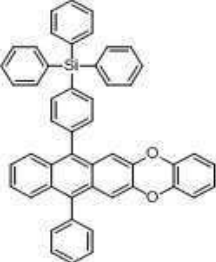
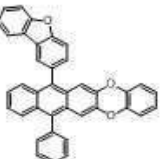
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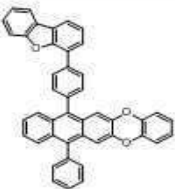
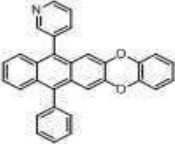
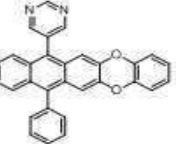
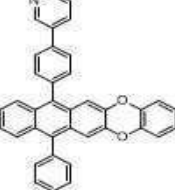
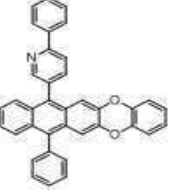
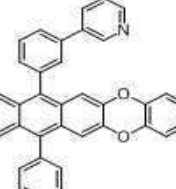
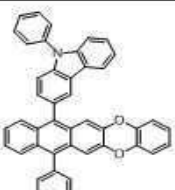
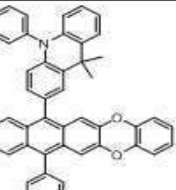
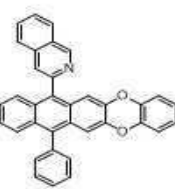
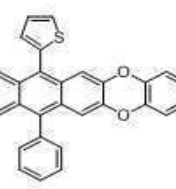
[0069]

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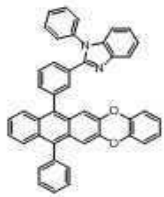
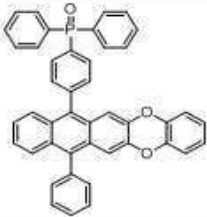
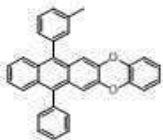
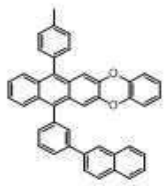
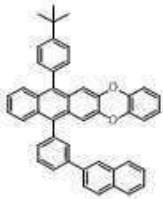
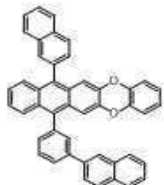
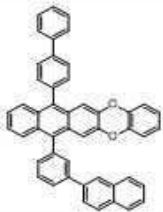
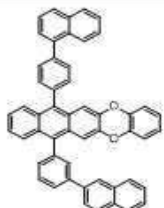
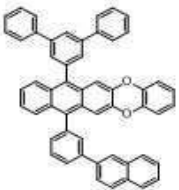
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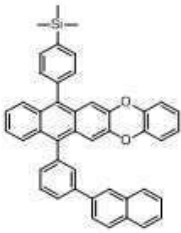
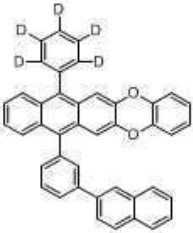
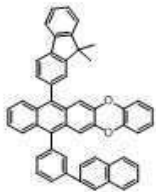
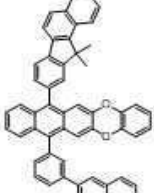
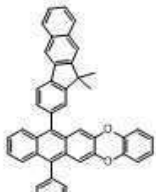
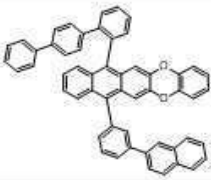
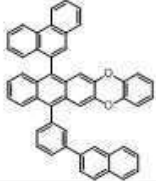
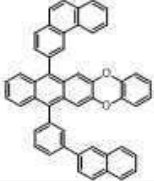
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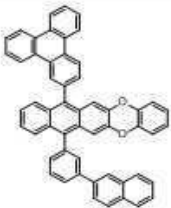
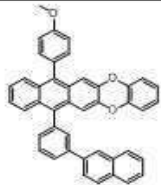
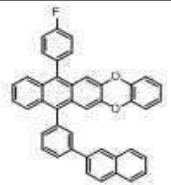
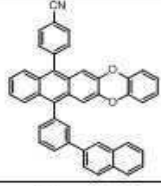
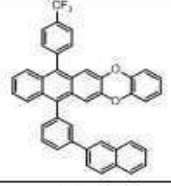
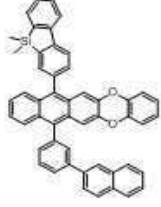
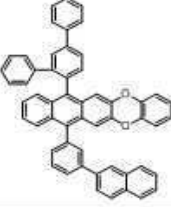
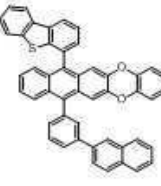
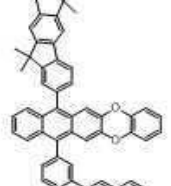
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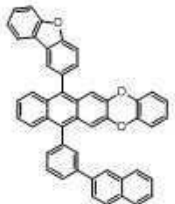
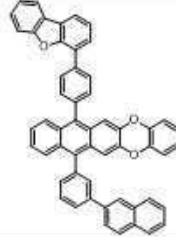
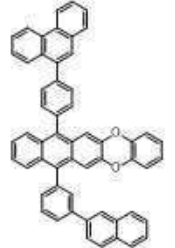
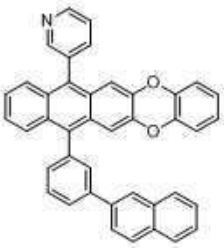
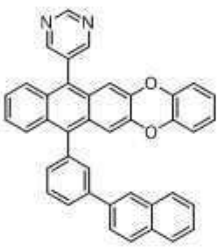
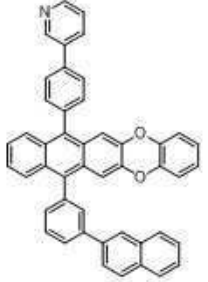
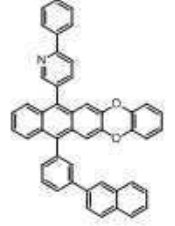
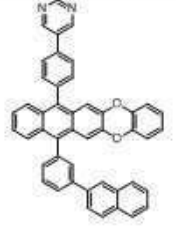
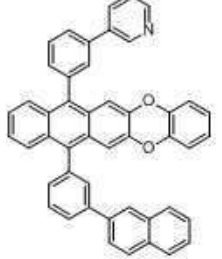
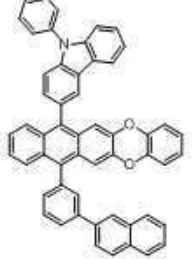
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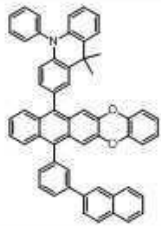
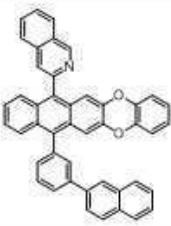
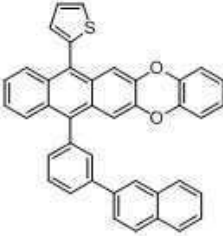
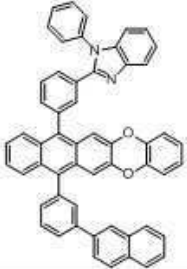
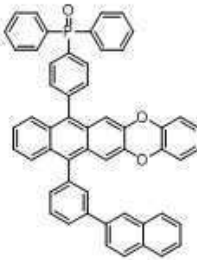
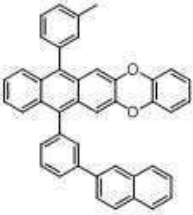
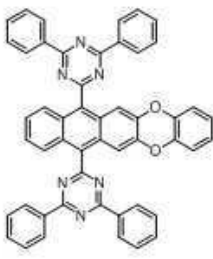
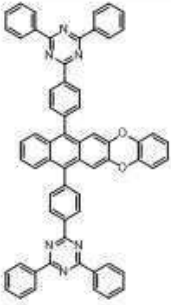
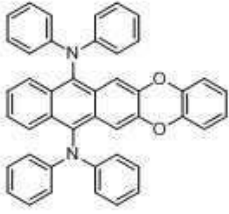
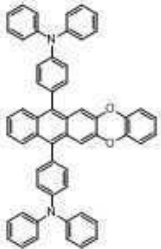
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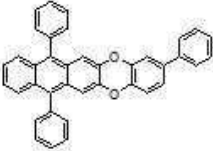
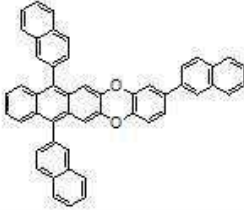
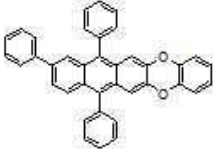
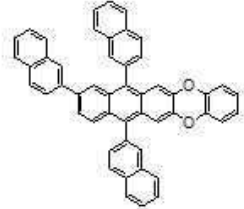
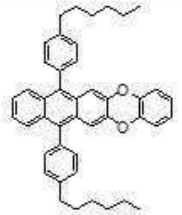
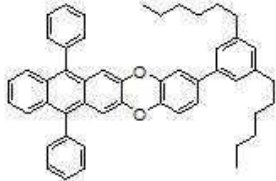
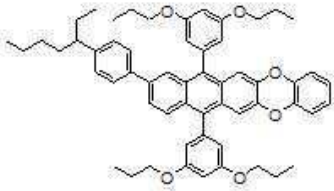
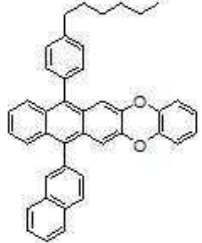
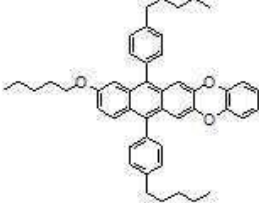
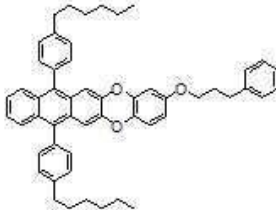
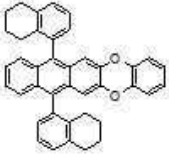
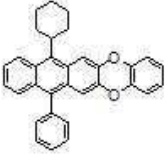
[0075]

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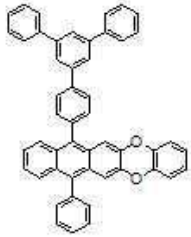
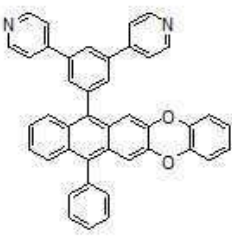
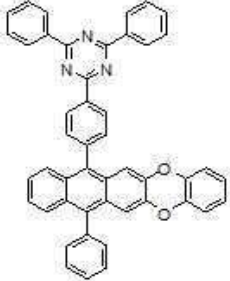
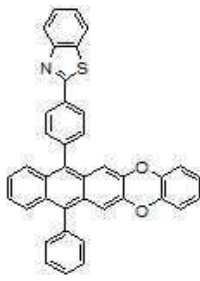
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[0078]

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[0079]

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[0080]

[0081] 본 발명의 다른 구현예에서, 상기 유기 발광 화합물의 적어도 1종을 포함하는 잉크 조성물을 제공한다.

[0082] 상기 잉크 조성물은 용매를 포함하는 용액 또는 현탁액일 수 있고, 상기 용매는 예를 들어, 아니솔, 디메틸 아니솔, 크실렌, o-크시렌, m-크시렌, p-크시렌, 톨루엔, 메틸렌, 메틸 벤조에이트, 다이옥산, 테트라하이드로퓨란, 메틸 테트라하이드로퓨란, 테트라하이드로피란, 테트라린, 베라트올, 클로로벤젠, N-메틸 피롤리돈, N,N-디메틸포름아마이드, 디메틸술폭사이드 및 이들의 조합으로 이루어진 군으로부터 선택된 하나를 포함할 수 있다.

[0083] 상기 잉크 조성물을 도포한 뒤 용매를 제거하여 성막함으로써 유기물층을 형성할 수 있다.

[0084] 상기 잉크 조성물은 안료 또는 염료를 더 포함할 수 있다.

[0085] 상기 잉크 조성물은 인광 도판트 또는 형광 도판트를 더 포함할 수 있다.

[0086] 본 발명의 또 다른 구현예에서, 제1 전극, 1층 이상의 유기물층 및 제2 전극이 적층된 구조를 포함하고, 상기 유기물층은 상기 유기 발광 화합물을 적어도 1종 포함하는 유기 발광 소자를 제공한다.

[0087] 상기 유기 발광 소자의 유기물층에 포함되는 상기 유기 발광 화합물은 상기 화학식 1로 표시되는 화합물이고, 그에 대한 상세한 설명은 전술한 바와 같다.

[0088] 상기 유기물층은 유기 박막층을 형성하거나 적층하는 공지된 제조 방법에 따라서 제조될 수 있거나, 또는, 상기 유기물층은 전술한 바와 같이, 상기 잉크 조성물을 이용하여 용액 공정으로 성막하여 제조될 수 있다.

[0089] 일 구현예에서, 상기 유기물층이 발광층을 포함하고, 상기 발광층이 상기 유기 발광 화합물을 포함할 수 있고, 상기 유기 발광 화합물은 발광층 중 인광 호스트, 형광 호스트, 인광 도판트, 또는 형광 도판트 재료로서 포함될 수 있다.

[0090] 상기 발광층은 상기 화학식 1로 표시되는 화합물, 이외에, 추가적으로, 공지된 재료의 인광 호스트, 형광 호스트, 인광 도판트, 또는 형광 도판트 재료를 더 포함할 수 있다.

[0091] 상기 유기물층은 필요한 용도에 따라서 적절히 정공수송층, 정공주입층, 정공차단층, 전자수송층, 전자주입층 및 전자차단층으로 이루어진 군으로부터 선택된 하나 이상을 포함할 수 있다.

[0092] 상기 정공수송층, 정공주입층, 정공차단층, 전자수송층, 전자주입층 및 전자차단층은, 각각, 공지된 물질을 사용하여 형성되거나, 상기 화학식 1로 표시되는 유기 발광 화합물을 1종 이상 포함할 수 있다.

[0093] 본 발명의 또 다른 구현예에서, 상기 유기 발광 소자를 포함하는 전자 기기를 제공한다.

[0094] 상기 유기 발광 소자는 다양한 응용분야에 적용될 수 있다. 예를 들어, 상기 유기 발광 소자가 적용된 상기 전자 기기는 유기 집적 회로 (O-IC), 유기 전계-효과 트랜지스터 (O-FET), 유기 박막 트랜지스터 (O-TFT), 유기 발광 트랜지스터 (O-LET), 유기 태양 전지 (O-SC), 유기 광학 검출기, 유기 광수용체, 유기 전계-켄치 소자 (O-FQD), 발광 전기화학 전지 (LEC), 유기 레이저 다이오드 (O-레이저) 또는 유기 발광 소자 (OLED)일 수 있다.

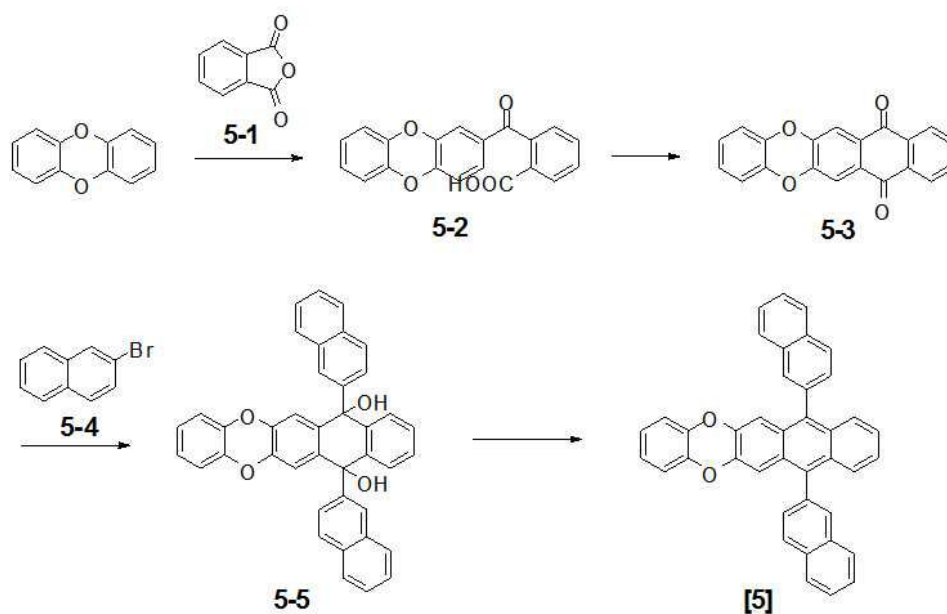
[0095] 이하 본 발명의 실시예 및 비교예를 기재한다. 그러한 하기한 실시예는 본 발명의 일 실시예일뿐 본 발명이 하기한 실시예에 한정되는 것은 아니다.

[0096] (실시예)

[0097] 이하에서, 반응예 및 비교예를 구체적으로 예시하지만, 본 발명이 하기의 합성예 및 실시예로 한정되는 것은 아니다. 이하의 반응예에서 중간체 화합물은 최종 생성물의 번호에 일련번호를 추가하는 방식으로 표기한다. 예를 들어, 화합물 1은 화합물 [1] 로 상기 화합물의 중간체 화합물은 [1-1] 등으로 표기한다. 본 명세서에서 화합물의 번호는 상기 표 1에 기재된 화학식의 번호로서 표기한다. 예를 들어, 표 1에서 1로 표시된 화합물은 화합물 1로 표기한다.

[0098] 합성예 1: 화합물 [5]의 제조

[0099] [반응식 1]



[0101] 중간체 화합물 [5-2]의 제조

[0102] 2L 반응플라스크에 질소 분위기에서 화합물 [5-1] 16.1g(108.58mmol)을 디클로로메탄 500ml에 녹이고, 염화알루미늄 28.9g(217.17mmol)을 넣고 30분간 교반하고, 디벤조-1,4-디옥신 20.0g(108.58mmol)을 적가하였다. 반응 종료 후 반응액을 얼음물에 적가한 후 디클로로메탄 100mL를 넣고 추출하여 무수황산 마그네슘으로 건조하여 여과하고, 여과액을 감압 농축한 뒤, 디클로로메탄 100ml에 녹여 헥산을 넣어 재결정하였다. 이를 여과하여 밝은 노란색 고체의 중간체 화합물 [5-2] 34.6g (96%)을 제조하였다.

[0103] 중간체 화합물 [5-3]의 제조

[0104] 500mL 반응플라스크에 질소 분위기에서 중간체 화합물 [5-2] 34.6g(104.12mmol)을 폴리인산에 녹이고 100℃로 가열 교반하였다. 반응 종료 후 반응액을 얼음물에 적가한 후 1시간 동안 교반시킨 후 감압 여과하였다. 그 후 고체를 아세톤 300ml와 증류수 1.5L를 가하여 교반 한 후 감압여과 하였다. 고체를 아세톤 600ml에 환류 교반한 후 감압여과하여, 갈색 고체의 중간체 화합물 [5-3] 28.8g (88%)을 제조하였다.

[0105] 중간체 화합물 [5-5]의 제조

[0106] 1L 반응플라스크에 화합물 [5-4] 49.3g(238.25mmol) 을 무수테트라히드로퓨란 500mL로 녹인 후 -78℃에서 교반 하였다. n-부틸리튬(2.5M in hexane) 95.3mL(238.25mmol)를 동온도에서 적가시키고 30분 후에 중간체 화합물 [5-3] 28.8g(91.63mmol)을 가하였다. 반응온도를 상온까지 올리고 에틸아세테이트와 포화암모늄 수용액으로 추출한 후 무수황산 마그네슘으로 건조하여 여과하고, 여과액을 감압 농축한 뒤 실리카겔 크로마토 그래프로 분리 정제하여, 밝은 노란색 고체의 중간체 화합물 [5-5] 24.2g(40%)을 제조하였다.

[0107] 화합물 [5]의 제조

[0108] 500mL 반응플라스크에 중간체 화합물 [5-5] 24.2g(42.4mmol), 요오드화 칼륨 28.2g(169.63mmol), 치아인산나트륨 1 수화물 36.0g(169.63mmol)을 넣고 아세트산 200ml 첨가 후 6시간 환류교반시켰다. 반응온도를 상온으로 냉각시키고 생성된 고체를 여과한다. 여과한 고체를 아세톤 200ml와 증류수 800ml를 가하여 1시간 동안 교반한 후 감압여과하였다. 여과된 고체를 톨루엔으로 재결정화하여, 연한 노란색 고체의 목적화합물 [5] 8.4g(37%)을 제조하였다.

[0109] ^1H NMR (400 MHz, THF- d_8): δ 8.18(d, 2H), 8.10~7.99(m, 6H), 7.66~7.61(m, 8H), 7.29~7.27(m, 2H), 7.12(s, 2H), 6.94~6.84(m, 4H)

[0110] MS/FAB : 536(M^+)

[0111] 도 1은 상기 얻은 화합물 [5]에 대한 ^1H -NMR 그래프이다.

[0112] 도 2는 상기 얻은 화합물 [5]에 대한 열중량분석 (thermogravimetric analysis, TGA) 그래프이다.

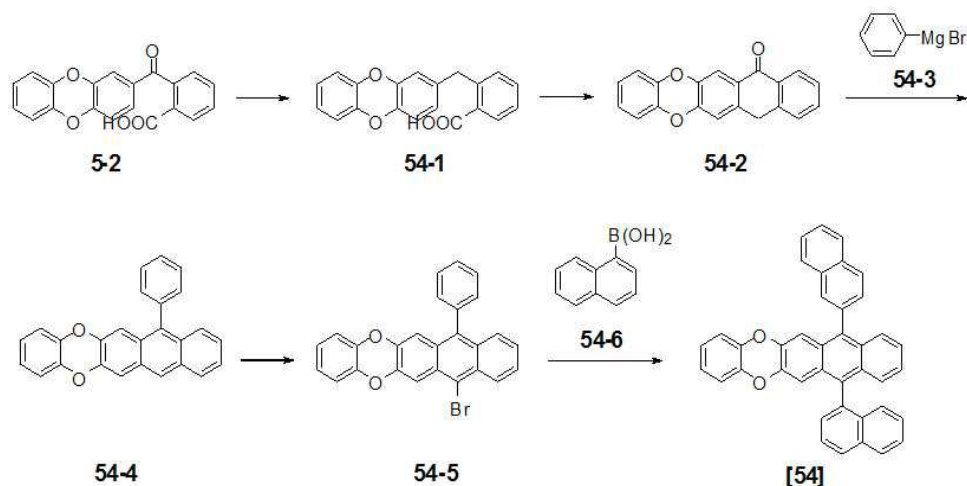
[0113] 도 3은 상기 얻은 화합물 [5]에 대한 시차주사열량 (differential scanning calorimetry, DSC) 측정 그래프이다.

[0114] 도 4는 상기 얻은 화합물 [5]에 대한 UV 흡수스펙트럼이다.

[0115] 도 5는 상기 얻은 화합물 [5]에 대한 광발광 (Photoluminescence, PL) 측정 그래프 이다.

[0116] 합성예 2: 화합물 [54]의 제조

[0117] [반응식 2]



[0118]

[0119] **중간체 화합물 [54-1]의 제조**

[0120] 1L 반응플라스크에 화합물 [5-2] 30g(90.28mmol), 아연 59.1g(902.77mmol), 수산화나트륨 36.1g(902.77mmol)에 디에틸글라이콜 600ml를 가하고 160℃에서 24시간 환류교반하였다. 반응 종료 후 증류수 100ml에 반응액을 천천히 부어주고 36% 염산을 적가하여 pH를 1-2정도로 만든 뒤, 1시간 실온 교반하였다. 감압 여과하여 고체를 얻고, 얻어진 고체에 디클로로메탄을 가하여 녹인 뒤, 실리카겔 크로마토그래프로 분리정제하여, 미색고체의 중간체 화합물 [54-1] 17.5g (61%)을 제조하였다.

[0121] **중간체 화합물 [54-2]의 제조**

[0122] 500mL 반응플라스크에 화합물 [54-1] 17.5g(54.98mmol)에 메탄술폰산 100ml을 넣고 질소 분위기에서 1시간 동안 실온 교반하였다. 그 뒤 100℃까지 반응기 온도를 천천히 올린 뒤 24시간 교반하였다. 반응 종료 후 증류수 100ml에 반응액을 천천히 부어주고 1시간 실온 교반한 뒤 디클로로메탄으로 추출하여 무수황산 마그네슘으로 건조하여 여과한다. 여과액은 감압 농축한 뒤, 실리카겔 크로마토그래프로 분리정제하여, 미색고체의 중간체 화합물 [54-2] 7.8g (47%)을 제조하였다.

[0123] **중간체 화합물 [54-4]의 제조**

[0124] 500ml 반응플라스크에 질소 분위기에서 중간체 화합물 [54-2] 7.8g(25.97mmol)에 테트라하이드로퓨란 100ml를 가한 후, 페닐 마그네슘 브로마이드(1.0M in THF) 77.9ml(77.92mmol)을 넣고 28시간 환류 교반하였다. 반응 종료 후 감압 여과하고, 여과된 반응액에 36% 염산을 적가하여 pH를 1-2로 맞추고 디클로로메탄으로 추출하여 무수황산 마그네슘으로 건조하여 여과하였다. 여과액은 감압 농축한 뒤, 디클로로메탄, 헥산, 메탄올을 이용하여 재결정하고, 얻어진 고체를 실리카겔 크로마토그래프로 분리정제하여, 밝은 미색 고체의 중간체 화합물 [54-4] 3.9g (42%)을 제조하였다.

[0125] **중간체 화합물 [54-5]의 제조**

[0126] 500ml 반응플라스크에 질소 분위기에서 중간체 화합물 [54-4] 3.9g(10.82mmol), N-브로모석신이미드 2.3g(12.99mmol)에 디클로로메탄 250ml를 가하고 10시간 실온에서 교반하였다. 반응 종료 후 디클로로메탄으로 추출하여 무수황산 마그네슘으로 건조하여 여과하고, 실리카겔 크로마토그래프로 분리정제하여, 밝은 노란색 고체의 중간체 화합물 [54-5] 3.9g (82%)을 제조하였다.

[0127] **화합물 [54]의 제조**

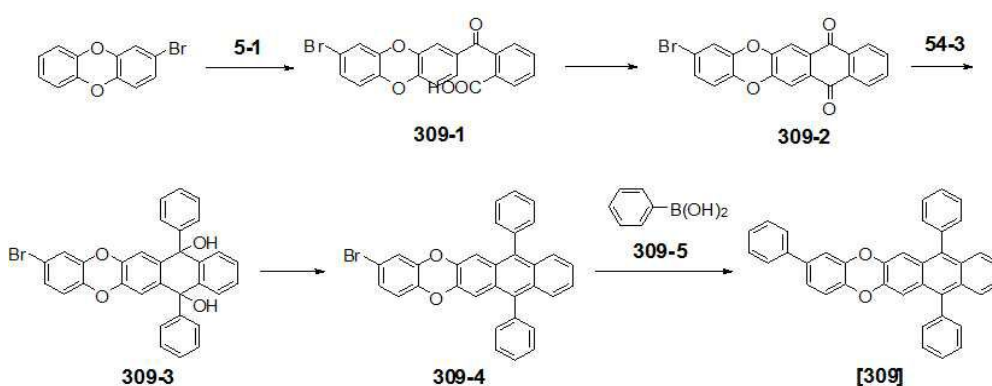
[0128] 250ml 반응플라스크에 중간체 화합물 [54-5] 3.9g(8.88mmol), 화합물 [54-6] 1.8g(10.65mmol), 테트라키스(트리페닐포스핀)팔라듐 0.31g(0.27mmol), 포타슘카보네이트 3.7g(26.63mmol), 증류수 30ml, 톨루엔 90ml를 가하고 24시간 환류 교반하였다. 반응 종료 후 디클로로메탄으로 추출하여 무수황산 마그네슘으로 건조하여 여과하고, 여과액은 감압 농축한 뒤, 실리카겔 크로마토그래프로 분리정제하여, 미색고체의 목적화합물 [54] 2.6g (54%)을 제조하였다.

[0129] ^1H NMR (400 MHz, THF- d_8): δ 8.55~8.42(m, 2H), 8.08~8.04(m, 2H), 7.90(d, 2H), 7.61~7.38(m, 10H), 7.15~7.12(m, 4H), 6.92(d, 2H)

[0130] MS/FAB: 486(M $^+$)

[0131] 합성예 3: 화합물 [309]의 제조

[0132] [반응식 3]



[0133]

[0134] 중간체 화합물 [309-1]의 제조

[0135] 화합물[5-1] 15.2g(102.62mmol), 염화알루미늄 27.4g(205.25mmol), 2-브로모디벤조[b,e][1,4]디옥신 30.0g(114.03mmol)을 [합성예 1]의 방법을 이용하여 밝은 노란색 고체의 중간체 화합물 [309-1] 34.2g (81%)을 제조하였다.

[0136] 중간체 화합물 [309-2]의 제조

[0137] 중간체 화합물 [309-1] 34.2g(83.17mmol)을 [합성예 1]의 방법을 이용하여 갈색 고체의 중간체 화합물 [309-2] 14.7g (45%)을 제조하였다.

[0138] 중간체 화합물 [309-3]의 제조

[0139] 중간체 화합물 [309-2] 14.7g(37.39mmol), 페닐 마그네슘 브로마이드(1.0M in THF) 97.2ml(97.20mmol)을 [합성예 2]의 방법을 이용하여 고체의 중간체 화합물 [309-3] 15.0g (73%)을 제조하였다.

[0140] 중간체 화합물 [309-4]의 제조

[0141] 중간체 화합물 [309-3] 15.0g(27.30mmol), 요오드화 칼륨 18.1g(109.21mmol), 치아인산나트륨 1 수화물 23.15g(218.42mmol)을 [합성예 1]의 방법을 이용하여 연한 노란색 고체의 중간체 화합물[309-4]를 5.9g(42%)을 제조하였다.

[0142] **화합물 [309]의 제조**

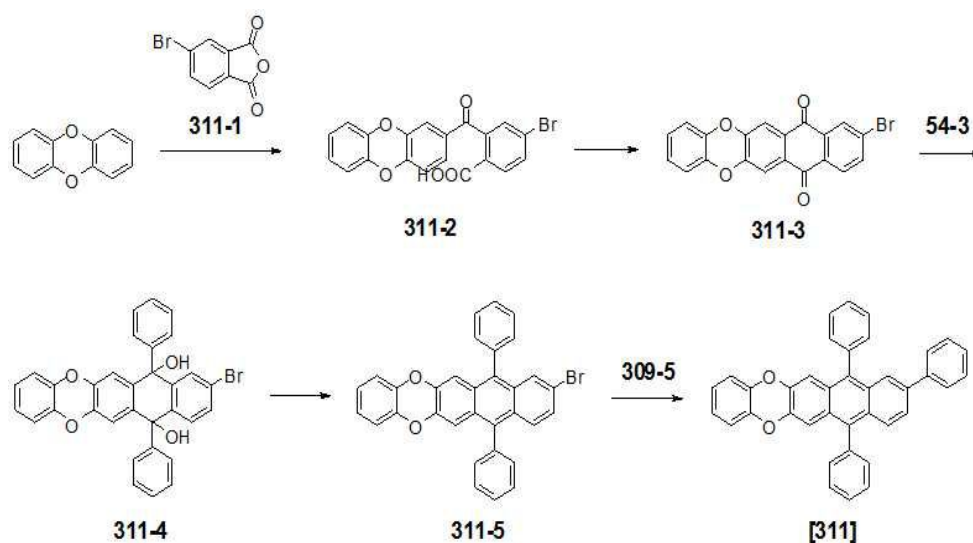
[0143] 중간체 화합물 [309-4] 5.9g(11.45mmol), 화합물 [309-5] 2.0g(16.03mmol), 테트라키스(트리페닐포스핀)팔라듐 0.40g(0.034mmol), 포타슘카보네이트 2.4g(17.17mmol)을 [합성예 2]의 방법을 이용하여 미색고체의 목적화합물 [309] 2.5g (43%)을 제조하였다.

[0144] ^1H NMR (400 MHz, THF- d_8): δ 7.90(d, 2H), 7.61~7.41(m, 19H), 7.20~7.17(m, 3H)

[0145] MS/FAB: 512(M⁺)

[0146] **합성예 4: 화합물 [311]의 제조**

[0147] [반응식 4]



[0149] **중간체 화합물 [311-2]의 제조**

[0150] 화합물[311-1] 33.3g(146.59mmol), 염화알루미늄 39.1g(293.18mmol), 디벤조-1,4-디옥신 30.0g(162.88mmol)을 [합성예 1]의 방법을 이용하여 밝은 노란색 고체의 중간체 화합물 [311-2] 47.0g (78%)을 제조하였다.

[0151] **중간체 화합물 [311-3]의 제조**

[0152] 중간체 화합물 [311-2] 47.0g(114.30mmol)을 [합성예 1]의 방법을 이용하여 갈색 고체의 중간체 화합물 [311-3] 27.9g (62%)을 제조하였다.

[0153] **중간체 화합물 [311-4]의 제조**

[0154] 중간체 화합물 [311-3] 27.9g(70.96mmol), 페닐 마그네슘 브로마이드(1.0M in THF) 184.5ml(184.50mmol)을 [합성예 2]의 방법을 이용하여 고체의 중간체 화합물 [311-4] 16.4g (42%)을 제조하였다.

[0155] **중간체 화합물 [311-5]의 제조**

[0156] 중간체 화합물 [311-4] 16.4g(29.85mmol), 요오드화 칼륨 19.8g(119.40mmol), 치아인산나트륨 1 수화물 25.3g(238.80mmol)을 [합성예 1]의 방법을 이용하여 연한 노란색 고체의 중간체 화합물[311-5]를 8.5g(55%)을 제조하였다.

[0157] **화합물 [311]의 제조**

[0158] 중간체 화합물 [311-5] 8.5g(16.49mmol), 페닐보론산 2.8g(23.09mmol), 테트라키스(트리페닐포스핀)팔라듐 0.57g(0.49mmol), 포타슘카보네이트 3.4g(24.74mmol)을 [합성예 2]의 방법을 이용하여 미색고체의 목적화합물 [311] 4.4g (52%)을 제조하였다.

[0159] ^1H NMR (400 MHz, THF- d_8): δ 8.15(s, 1H), 7.92(d, 1H), 7.65(d, 1H), 7.56~7.43(m, 15H), 7.20~7.17(m, 4H), 6.92(d, 2H)

[0160] MS/FAB: 512(M⁺)

[0161] **합성예 5-10**

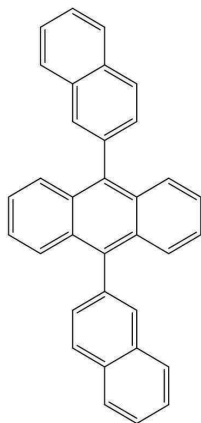
[0162] 상기 합성예 1-4에서 치환기만 대체한 적절한 화합물을 사용하여 화합물 [121], 화합물 [153], 화합물 [178], 화합물 [196], 화합물 [213] 및 화합물 [247]을 합성하였다.

[0163] **비교예 1**

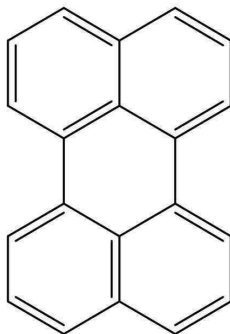
[0164] 하기 화학식 a로 표시되는 화합물 a를 형광 청색 호스트로 사용하고, 하기 화학식 b로 표시되는 화합물 b를 형광 청색 도판트로 사용하고, 2-TNATA(4,4',4"-tris(N-naphthalen-2-yl)-N-phenylamino)-triphenylamine)을 정공주입층 물질로 사용하고, α -NPD(N,N'-di(naphthalene-1-yl)-N,N'-diphenylbenzidine)을 정공수송층 물질로 사용하여, 다음과 같은 구조를 갖는 유기 발광 소자를 제작하였다: ITO/2-TNATA(80 nm)/ α -NPD(30 nm)/화학식a+화학식b(30 nm)/Alq₃(30 nm)/Liq(1 nm)/ Al(100 nm).

[0165] 애노드는 코닝(Corning)사의 $15\Omega/\text{cm}^2$ (1000Å) ITO 유리 기판을 25 mm x 25 mm x 0.7 mm크기로 잘라서 아세톤 이소프로필 알콜과 순수한 물 속에서 각 15분 동안 초음파 세정한 후, 30분 동안 UV 오존 세정하여 사용하였다. 상기 기판 상부에 2-TNATA를 진공 증착하여 80 nm 두께의 정공주입층을 형성하였다. 상기 정공주입층 상부에, α -NPD를 진공 증착하여 30 nm 두께의 정공수송층을 형성하였다. 상기 정공수송층 상부에 화학식 a로 표시되는 화합물 및 화학식 b로 표시되는 화합물(도핑률: 5%)를 진공 증착하여 30 nm두께의 발광층을 형성하였다. 이후, 상기 발광층 상부에 Alq₃ 화합물을 30 nm의 두께로 진공증착하여 전자수송층을 형성하였다. 상기 전자수송층 상부에 Liq 1 nm(전자주입층)과 Al 100 nm(캐소드)를 순차적으로 진공증착하여, 표 1에 표시된 바와 같은 유기 발광소자를 제조하였다. 이를 비교샘플 1이라고 한다.

<화학식 a>



<화학식 b>



[0166]

[0167] 실시예 1~10

[0168] 상기 비교 예 1 중에서, 형광 청색 호스트 화학식 a 대신 상기 합성예에 개시된 화합물 5, 54, 121, 153, 178, 196, 213, 247, 309 및 311을 형광 청색 호스트로 각각 이용한 것을 제외하고는 상기 비교예 1과 동일한 방법으로 ITO/2-TNATA(80nm)/ α -NPD(30 nm)/ 화합물 5, 54, 121, 153, 178, 196, 213, 247, 309 또는 311 + 화학식 b(5%)](30 nm)/Alq₃(30 nm)/Liq(1 nm)/Al(100 nm)의 구조를 갖는 유기발광소자를 제조하였다. 이를 각각 샘플 1 내지 10 이라고 한다.

[0169] 평가예 1: 비교샘플 1 및 샘플 1~10의 발광 특성 평가

[0170] 비교샘플 1 및 샘플 1~10 에 대하여, Keithley sourcemeter "2400", KONIKA MINOLTA "CS-2000"을 이용하여 발광휘도, 발광효율, 발광피크를 각각 평가하여, 그 결과를 하기 표 2에 나타내었다. 상기 샘플들은 456~463nm 범위에서 청색 발광 피크 값을 보여주었다.

표 2

[0171]

샘플 No.	형광 청색 호스트 No.	형광 청색 도판트 No.	전압 OP. V	휘도 [cd/m ²]	효율 [cd/A]	발광피크 [nm]
비교샘플 1	a	b	5.12	435	4.35	456, 484
1	5	b	4.8	550	5.50	461
2	54	b	4.5	533	5.33	462
3	121	b	4.3	523	5.23	461
4	153	b	4.4	514	5.14	459
5	178	b	4.8	489	4.89	462
6	196	b	4.4	501	5.01	458
7	213	b	4.7	499	4.99	458
8	247	b	4.6	501	5.01	459
9	309	b	4.6	532	5.32	459
10	311	b	4.7	546	5.56	469

[0172] 상기 표 2에 보여지는 바와 같이 샘플 1~10 은 비교샘플 1 에 비하여 향상된 발광 특성을 나타내었다.

[0173] **평가예 2: 비교샘플 1 및 샘플 1 ~ 10의 수명 특성 평가**

[0174] 비교샘플 1 및 샘플 1 ~ 10 에 대하여, ENC technology사의 LTS-1004AC 수명측정장치를 이용하여 700 nit를 기준으로 수명이 97%에 도달하는 시간을 각각 측정하여, 그 결과를 하기 표 3에 나타내었다.

표 3

[0175]

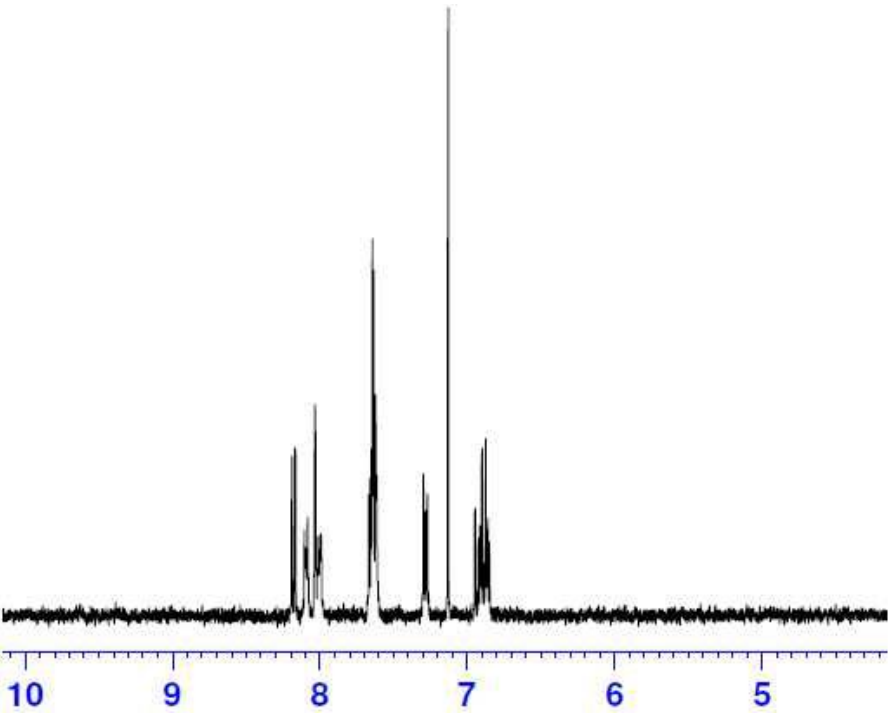
샘플 No.	형광 청색 호스트 No.	형광 청색 도판트 No.	수명 Time[Hours]
비교샘플 1	a	b	45
1	5	b	73
2	54	b	75
3	121	b	69
4	153	b	67
5	178	b	84
6	196	b	63
7	213	b	75
8	247	b	68
9	309	b	71
10	311	b	62

[0176] 상기 표 3에 보여지는 바와 같이 샘플 1~10 는 비교샘플 1 에 비하여 향상된 수명 특성을 나타내었다.

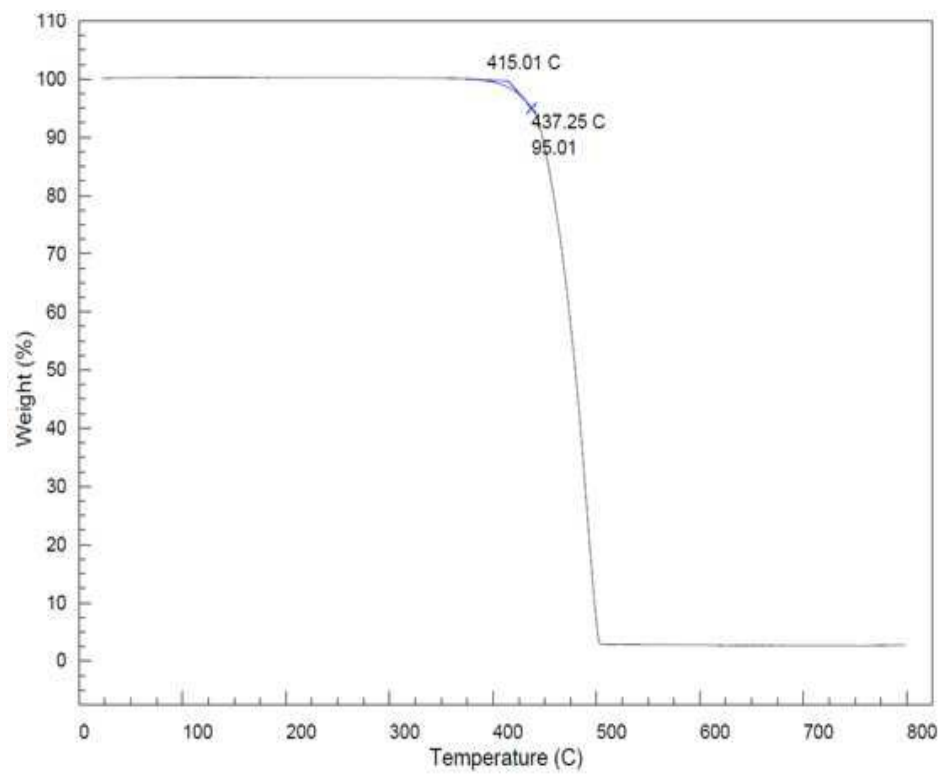
[0177] 이상에서 본 발명의 바람직한 실시예들에 대하여 상세하게 설명하였지만 본 발명의 권리 범위는 이에 한정되는 것은 아니고 다음의 청구 범위에서 정의하고 있는 본 발명의 기본 개념을 이용한 당업자의 여러 변형 및 개량 형태 또한 본 발명의 권리 범위에 속하는 것이다.

도면

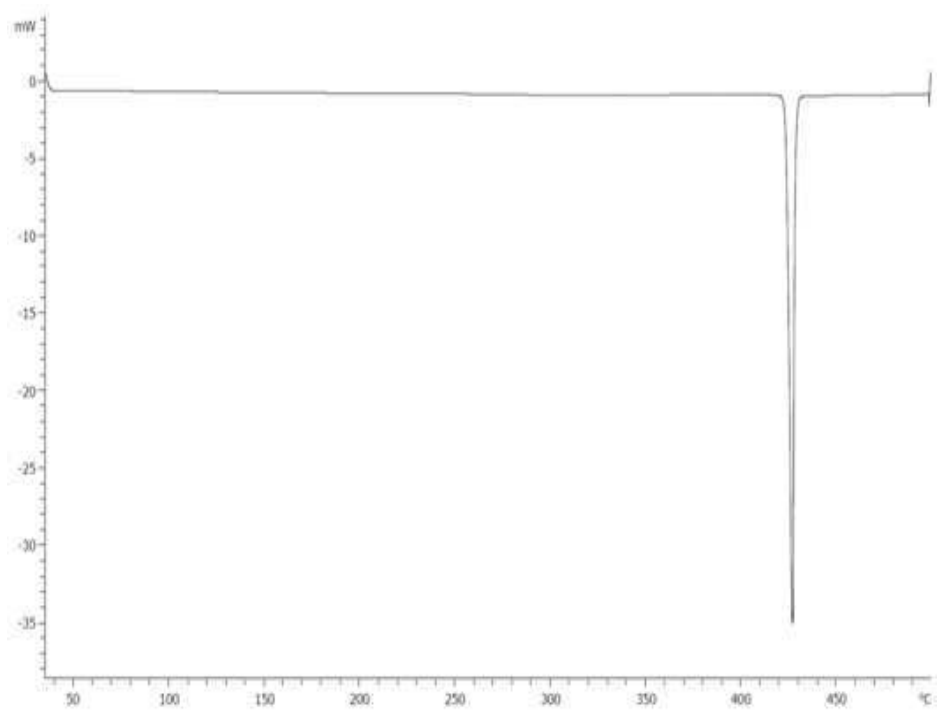
도면1



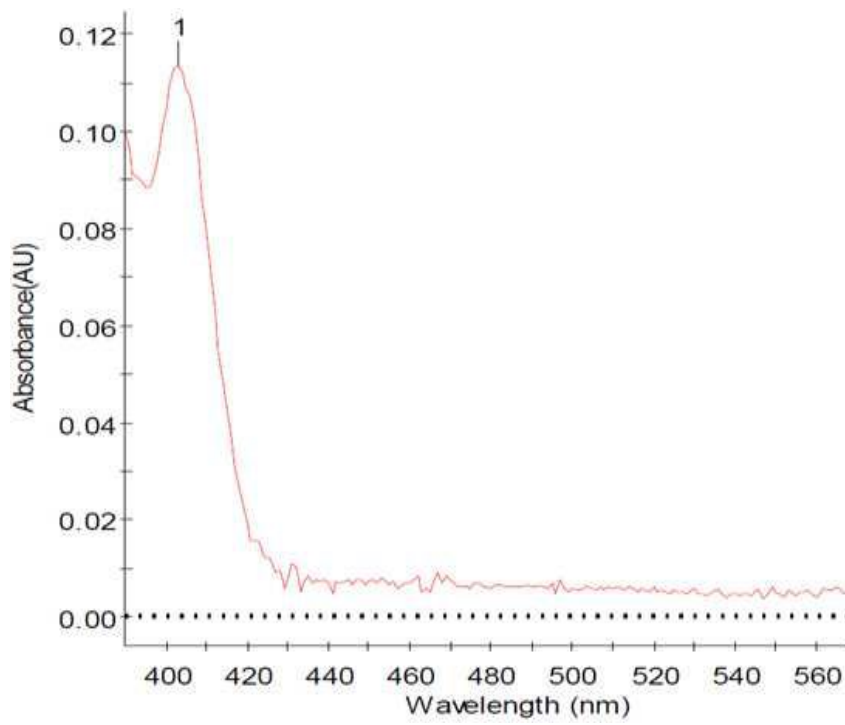
도면2



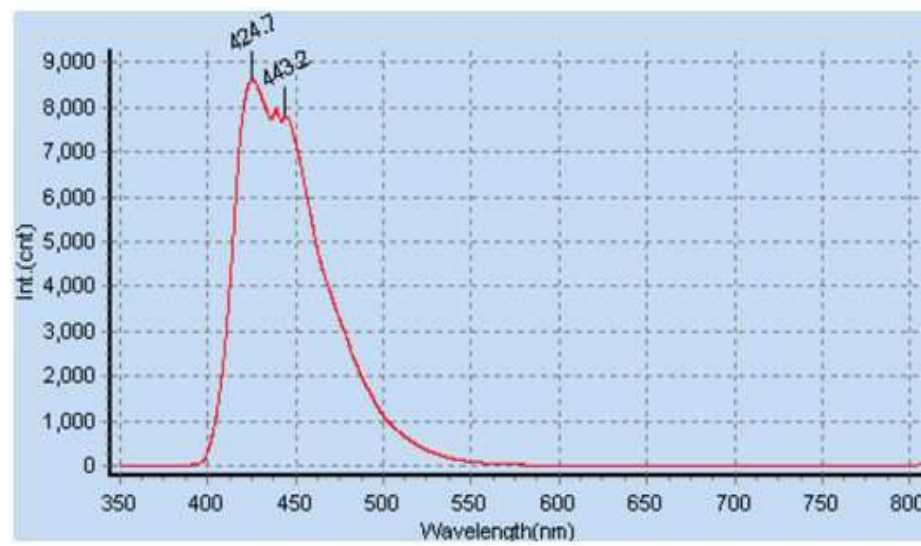
도면3



도면4



도면5



专利名称(译)	标题：有机发光化合物，油墨组合物，有机发光器件和电子器件		
公开(公告)号	KR101764913B1	公开(公告)日	2017-08-04
申请号	KR1020140147744	申请日	2014-10-28
申请(专利权)人(译)	氛围有限公司凯		
当前申请(专利权)人(译)	(株) M.L		
[标]发明人	GYUNG WOO KIM 김경우 HA NA SEO 서하나 DO HWAN AHN 안도환 DAE KYUN LEE 이대균 SO YEON KIM 김소연 MIN YOUNG OH 오민영 JUN SU AHN 안준수 KYUNG CHUL SHIN 신경철 HYUN CHUL LIM 임현철 YONG GU HONG 홍용구 HO GI BAE 배호기 JUNG BOK AN 안중복		
发明人	김경우 서하나 안도환 이대균 김소연 오민영 안준수 신경철 임현철 홍용구 배호기 안중복		
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其他公开文献	KR1020160049923A		
外部链接	Espacenet		

摘要(译)

提供由下式 (1) 表示的有机发光化合物。 钟铉啊 <式1> 1 2 1 2
其中Ar , Ar , L , L , Ra , Rb , n和m如上所定义。

