(19)国家知识产权局

(12)发明专利

(10)授权公告号 CN 111925366 B
(45)授权公告日 2024.04.09

(21)申请号 201910393579.5

(22)申请日 2019.05.13

(65)同一申请的已公布的文献号
申请公布号 CN 111925366 A

(43)申请公布日 2020.11.13

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(51)Int.Cl.
C07D 471/04(2006.01)
C07D 519/00(2006.01)
C09K 11/06(2006.01)
H10K 85/60(2023.01)

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审查员 王欢

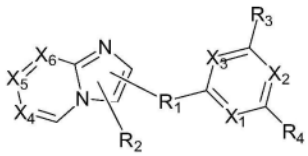
权利要求书5页 说明书33页

(54)发明名称

一种咪唑并氮杂环化合物及其应用

(57)摘要

本发明涉及一种咪唑并氮杂环化合物及其应用。本发明化合物具有式I所示结构。本发明咪唑并氮杂环化合物具有升华温度低,光、电、热稳定性好,折射率高、可见光区折射率差异小等优点,该化合物制备的器件具有电压低、寿命长,发光效率高等优点,可用于有机发光器件中。特别是作为电子传输材料、空穴阻隔层材料、光提取层材料,具有应用于AMOLED产业的可能。



(I)

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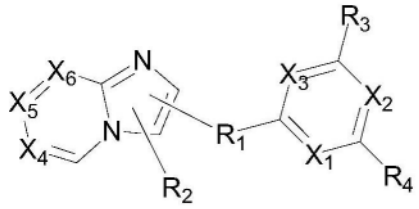
1.一种化合物,其结构式如式(I)所示:



（I）

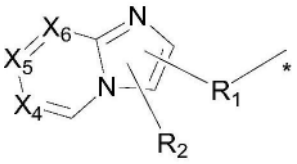
其中X1为N,X2、X3独立的表示为CH;或者X_1为CH,X_2、X_3独立的表示为N;或者X_1、X_2、X_3独立的表示为N;

X_4、X_5、X_6独立的表示为CR_0,R_0独立的选自氢;

其中X_1、X_2、X_3至少一个是N,其中R_4为式(II)结构,R_3为C1-C4烷基取代或未取代的C6-C18的芳基,

R_1为C1-C4烷基取代或未取代的C6-C18的非稠环芳基,

R_2为C1-C4烷基取代或未取代的C6-C18的芳基;



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式（II ）

2.根据权利要求1所述的化合物,其中R_1为C6-C18的非稠环芳基;R_2为C6-C18的芳基。

3.根据权利要求2所述的化合物,为下列化合物之一:

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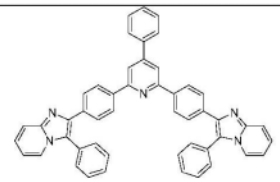
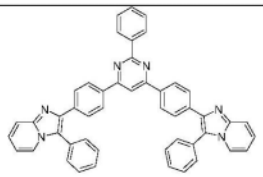
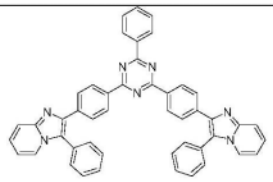
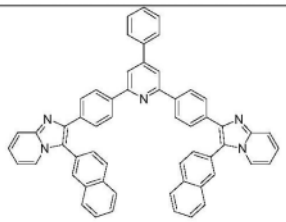
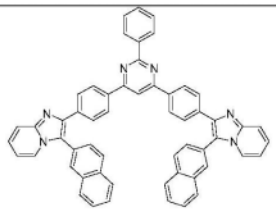
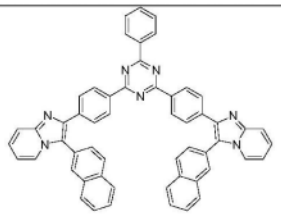
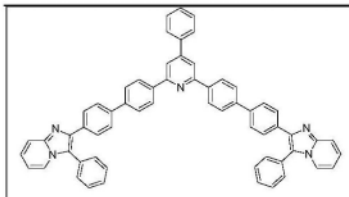
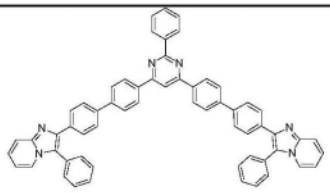
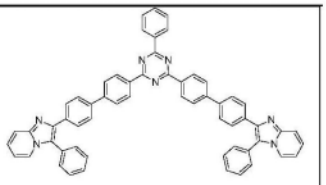
		
A 4	A 5	A 6
		
A 7	A 8	A 9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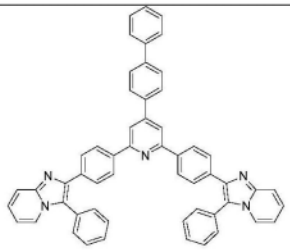	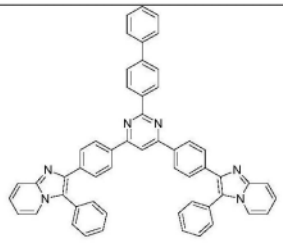	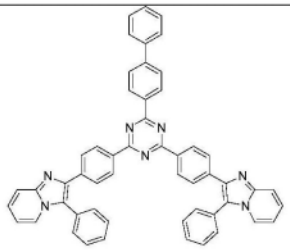
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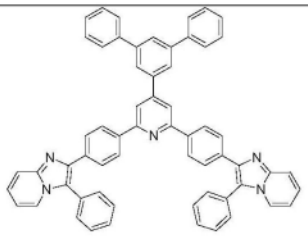	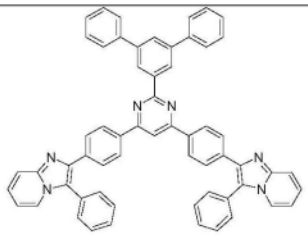	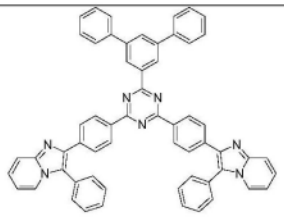
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		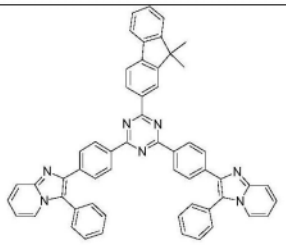
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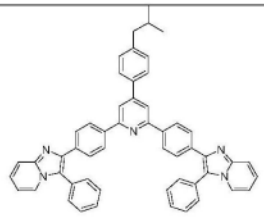	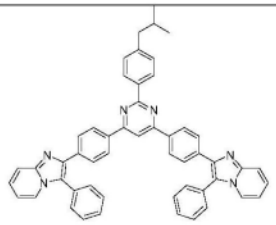	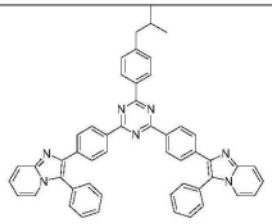
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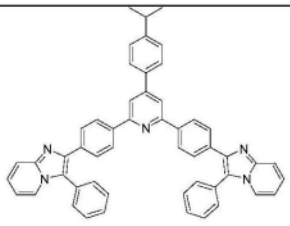	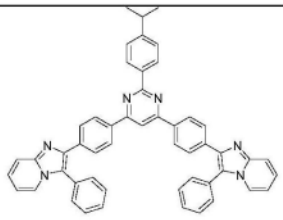	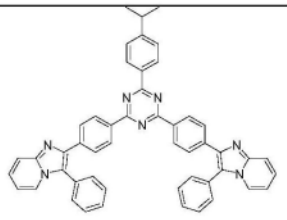

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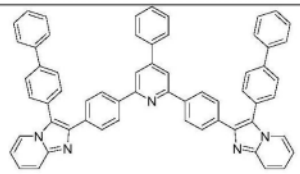	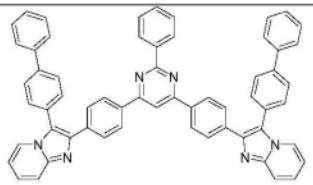	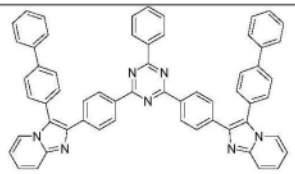
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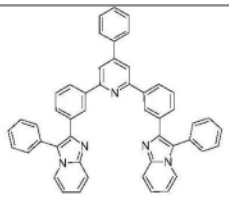	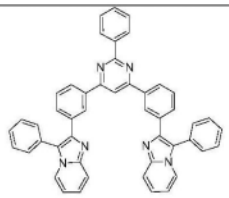	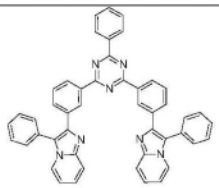
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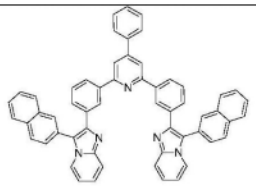	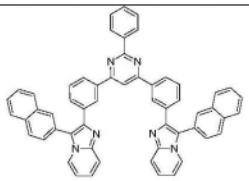	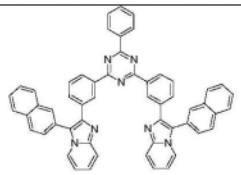
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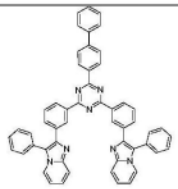	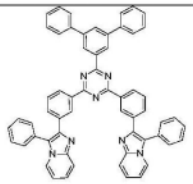	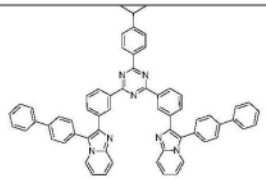
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		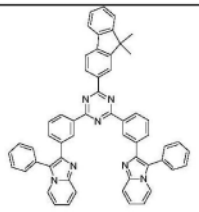
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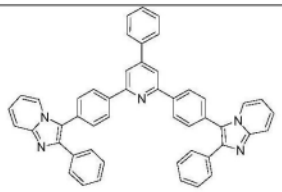	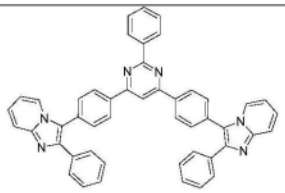	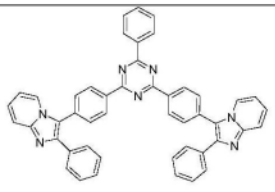
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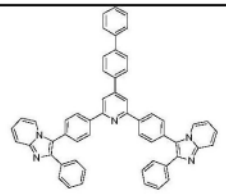	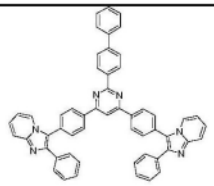	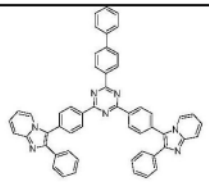
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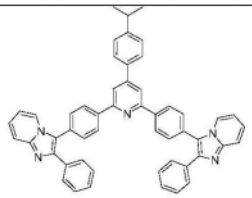	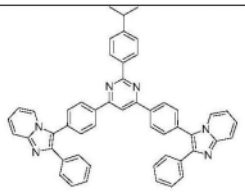	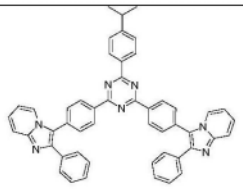
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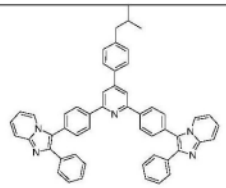	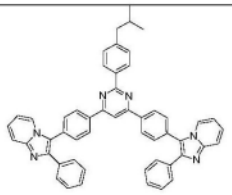	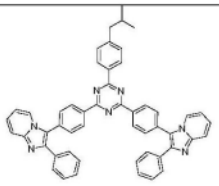
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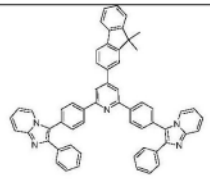	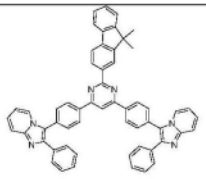	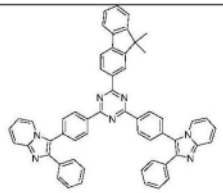
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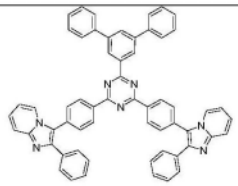	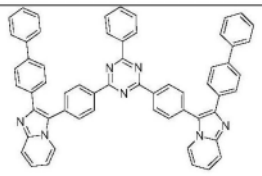	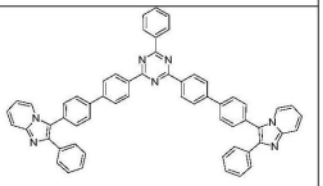
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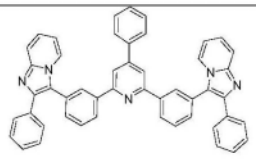	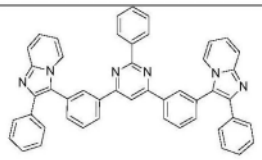	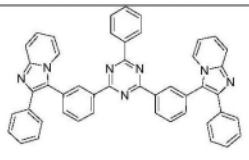
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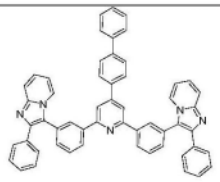	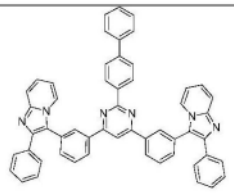	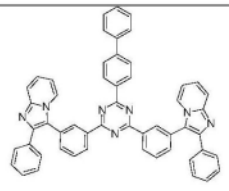

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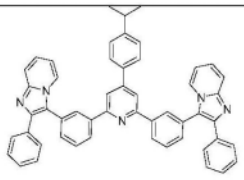
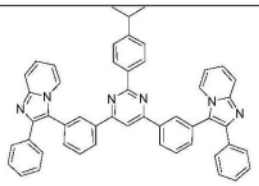
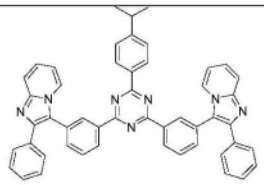
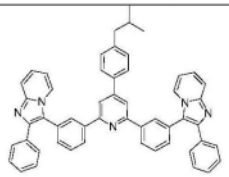
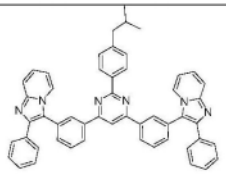
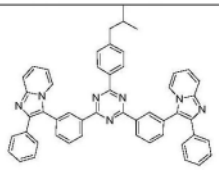
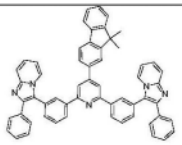
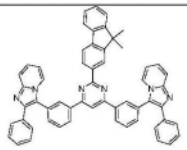
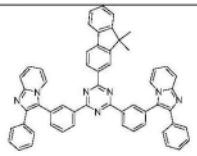
		
A 82	**A 83**	**A 84**
		
A 91	**A 92**	**A 93**
		
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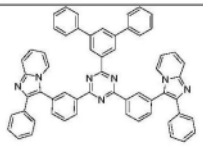
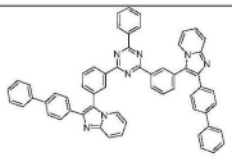
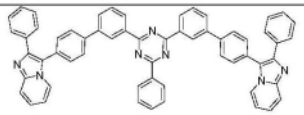
		

。

4.权利要求1-3任一项所述化合物在OLED器件中的应用;其特征在于:权利要求1-3任一项所述化合物作为OLED器件的电子传输层材料、空穴阻隔层材料和/或光提取层材料。

一种咪唑并氮杂环化合物及其应用

技术领域

[0001] 本发明涉及有机电致发光材料技术领域,特别涉及咪唑并氮杂环化合物及其在有机电致发光器件上的应用。

背景技术

[0002] 目前,作为新一代显示技术的有机电致发光器件(OLED)在显示和照明技术方面都获得了越来越多的关注,应用前景十分广泛。但是,和市场应用要求相比,OLED器件的发光效率、驱动电压、使用寿命等性能还需要继续加强和改进。

[0003] 一般来说,OLED器件基本结构为在金属电极中间夹杂各种不同功能的有机功能材料薄膜,犹如一个三明治的结构,在电流的驱动下,从阴阳两极分别注入空穴和电子,空穴和电子在移动一段距离后,在发光层得到复合,并以光或热的形式进行释放,从而产生了OLED的发光。然而,有机功能材料是有机电致发光器件的核心组成部分,材料的热稳定性、光化学稳定性、电化学稳定性、量子产率、成膜稳定性、结晶性、色饱和度等都是影响器件性能表现的主要因素。

[0004] 一方面,如何缩小OLED器件内外量子效率之间的巨大差距,如何减少器件中的全发射效应、提高光耦合提取比例引起人们的广泛关注。现行的光提取层的材料的折射率都比较低,尤其是在红光波段,通常折射率小于1.85,极少数大于1.90,更少数大于2.0。另外,现有的光提取材料在红绿蓝光波段区域的折射率差别较大,造成三种颜色光的最佳厚度差别大,未能充分体现光提取材料的性能。对于顶发射器件来说,光提取层材料的折射率越大,相应的外量子效率就越高,器件的发光效率就越高。所以,开发高折射率的光提取层材料尤为重要。CN103828485和TW201506128公开了以多联苯二胺为核心的光提取层材料,但是折射率还是稍微偏低,尤其是在红光方面更需要进一步提升。

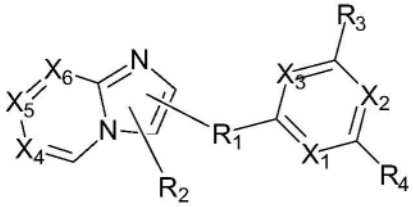
[0005] 另一方面,如何降低器件工作电压、降低产品功耗、提高器件寿命、提高发光效率,也是OLED器件不断提升的方向。CN101186608公开了一例以咪唑并吡啶和蒽环键接的化合物,这类化合物三线态能级、玻璃化转变温度和器件寿命都需要得到改善。邱等在CN103709180、CN103709181、CN103788087、CN103788116公开了一系列以咪唑并吡啶和稠合芳环键接的化合物,这类化合物的三线态能级、玻璃化转变温度和器件寿命也需要进一步改善。

发明内容

[0006] 针对上述领域中的缺陷,本发明提供一种咪唑并氮杂环化合物,所述化合物具有式I所示结构。该类化合物具有升华温度低,光、电、热稳定性好,折射率高、可见光区折射率差异小等优点,可用于有机发光器件中。

[0007] 本发明还提供该咪唑并氮杂环化合物在OLED中的应用,特别是作为电子传输材料、空穴阻隔层材料、光提取层材料,使器件具有发光效率高,电压低、寿命长的特点,具有应用于AMOLED产业的可能。

[0008] 一种化合物,其结构式如式(I)所示:

[0009] 

(I)

[0010] 其中R_1为单键、烷基、杂烷基、环烷基、取代或未取代的C6-C30的非稠环芳基、取代或未取代的C3-C27的非稠环杂芳基;

[0011] 其中R2、R3、R4独立的选自氢、氘、卤素、烷基、杂烷基、环烷基、烷氧基、芳氧基、氨基、硅烷基、腈、异腈、膦基、取代或未取代的C6-C60的芳基、取代或未取代的C1-C60的杂芳基、经取代或未经取代的单环或多环C3-C60脂肪族环或芳香族环且R3、R4中至少有一个为取代或未取代的C6-C60的芳基、取代或未取代的C1-C60的杂芳基、经取代或未经取代的单环或多环C3-C60脂肪族环或芳香族环,其中杂烷基或杂芳基中的一个或多个碳原子可由选自O、S、N、Se、Si、Ge中的至少一个杂原子替换;所述取代为被氘、卤素、C1-C30烷基、C1-C30杂烷基、C3-C30环烷基、氨基、硅烷基、腈、异腈、、膦基、C6-C60的芳基、C1-C60的杂芳基取代;

[0012] 其中X1、X2、X3独立的表示为CH或者N;X4、X5、X6独立的表示为CR_0或者N,R_0独立的选自氢、氘、卤素、烷基、杂烷基、芳烷基、烷氧基、芳氧基、氨基、硅烷基、芳基、杂芳基、腈、异腈、膦基,且相邻的R_0能键接成并环。

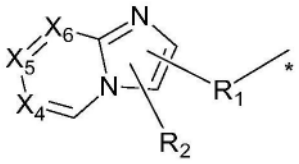
[0013] 优选:其中R_1为单键、C1-C30烷基、C1-C30杂烷基、C3-C30环烷基、取代或未取代的C6-C30的非稠环芳基、取代或未取代的C3-C27的非稠环杂芳基;

[0014] 其中R2、R3、R4独立的选自氢、氘、卤素、C1-C30烷基、C1-C30杂烷基、C3-C30环烷基、氨基、硅烷基、腈、异腈、膦基、取代或未取代的C6-C60的芳基、取代或未取代的C1-C60的杂芳基、经取代或未经取代的单环或多环C3-C60脂肪族环或芳香族环且R3、R4中至少有一个为取代或未取代的C6-C60的芳基、取代或未取代的C1-C60的杂芳基、经取代或未经取代的单环或多环C3-C60脂肪族环或芳香族环,其中杂烷基或杂芳基中的一个或多个碳原子由选自O、S、N中的至少一个杂原子替换;所述取代为被氘、卤素、C1-C30烷基、C1-C30杂烷基、C3-C30环烷基、氨基、硅烷基、腈、异腈、、膦基、C6-C60的芳基、C1-C60的杂芳基取代;

[0015] 其中X1、X2、X3独立的表示为CH或者N;X4、X5、X6独立的表示为CR_0或者N,R_0独立的选自氢、氘、卤素、C1-C30烷基、C1-C30杂烷基、芳烷基、氨基、硅烷基、芳基、杂芳基、腈、异腈、膦基,且相邻的R_0能键接成并环。

[0016] 进一步优选:其中X1、X2、X3至少一个是N。

[0017] 再优选:其中R3或R4至少之一含有以下结构式(II),其中R_1为单键、烷基、杂烷基、环烷基、C1-C30烷基取代或未取代的C6-C30的非稠环芳基、C1-C30烷基取代或未取代的C3-C27的非稠环杂芳基;其中R_2为氢、氘、卤素、烷基、杂烷基、环烷基、C1-C30烷基取代或未取代的C6-C60的芳基、C1-C30烷基取代或未取代的C1-C60的杂芳基

[0018]  。

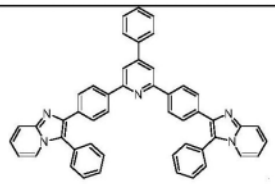
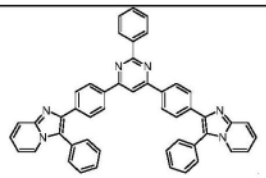
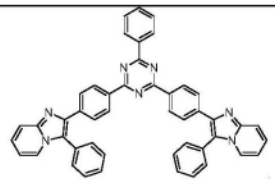
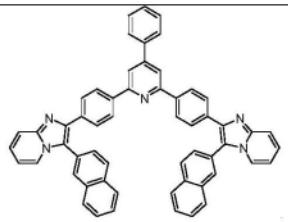
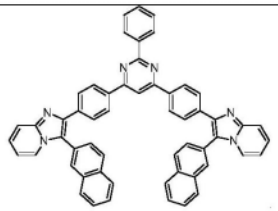
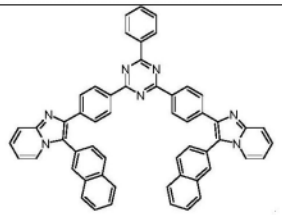
式（II）

[0019] 更优选:其中R3、R4中一个为式(II)结构,另一个为C1-C4烷基取代或未取代的C6-C18的芳基、C1-C4烷基取代或未取代的C3-C15的杂芳基;R1为C1-C4烷基取代或未取代的C6-C18的非稠环芳基、C1-C4烷基取代或未取代的C3-C15的非稠环杂芳基;R2为C1-C4烷基取代或未取代的C6-C18的芳基、C1-C4烷基取代或未取代的C3-C15的杂芳基。

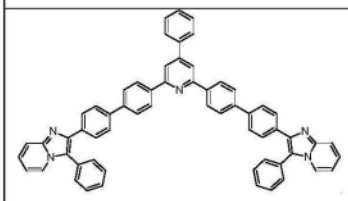
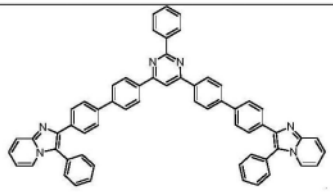
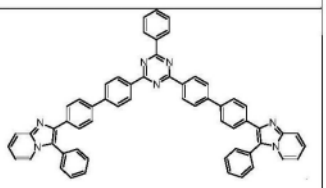
[0020] 优选:根据权利要求5所述的化合物,其中R1为C6-C18的非稠环芳基或C5-C15的非稠环杂芳基;R2为C6-C18的芳基或C5-C15的杂芳基。

[0021] 作为优选的化合物为以下化合物:

[0022]

A 1	A 2	A 3
		
A 4	A 5	A 6
		

[0023]

A 7	A 8	A 9
		
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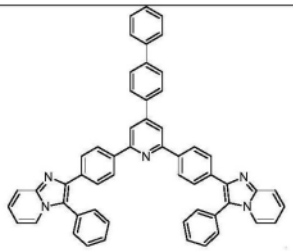	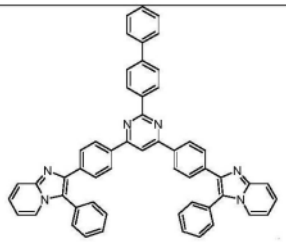	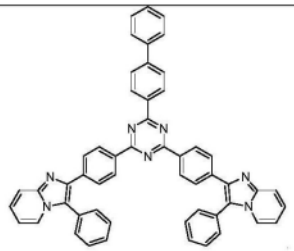
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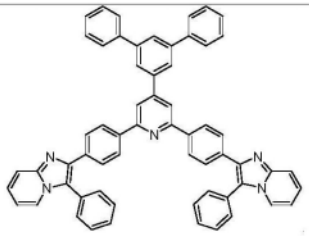	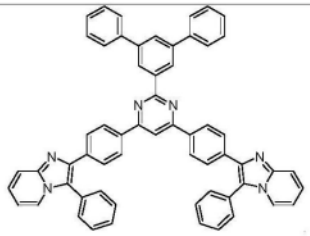	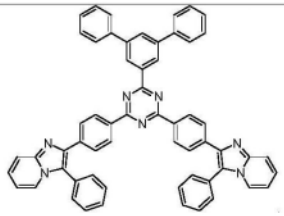
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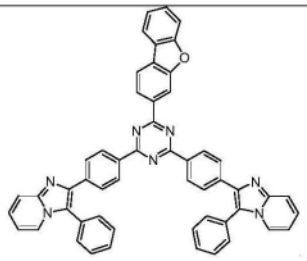	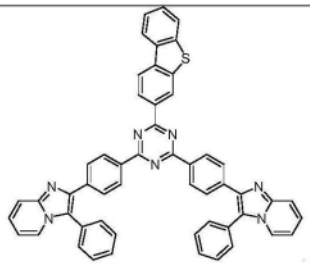	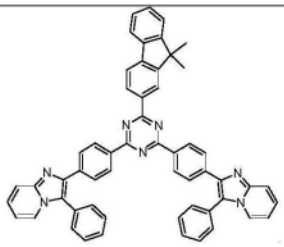
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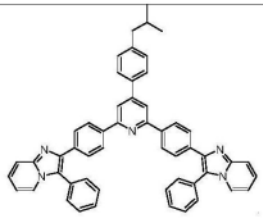	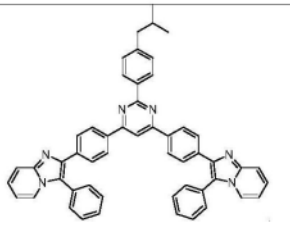	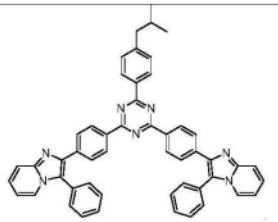
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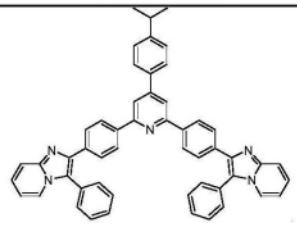	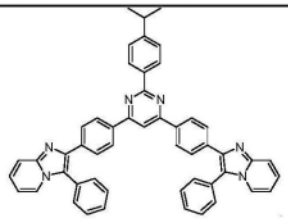	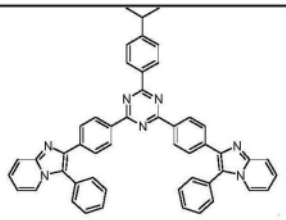
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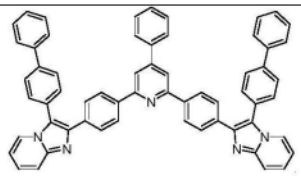	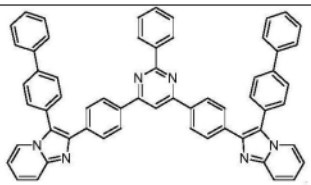	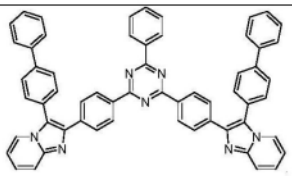
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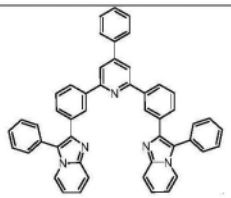	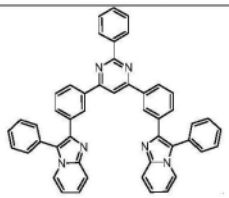	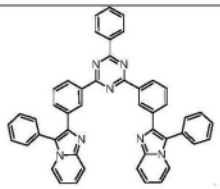
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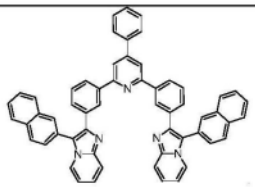	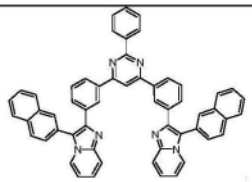	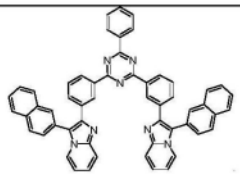
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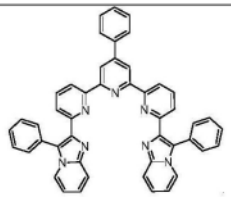	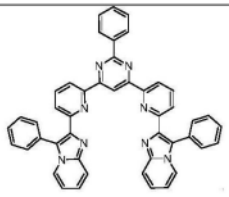	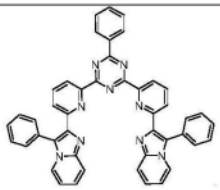
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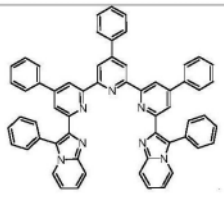	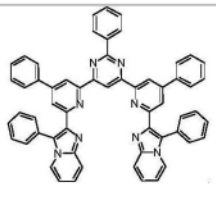	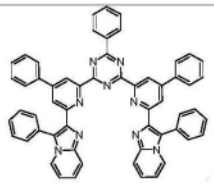
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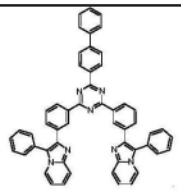	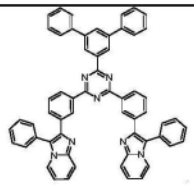	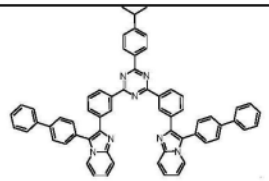
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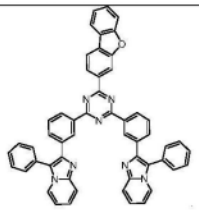	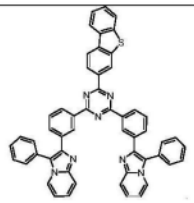	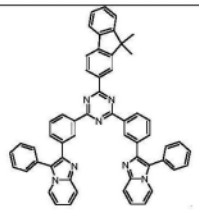
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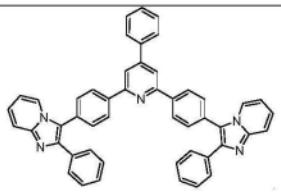	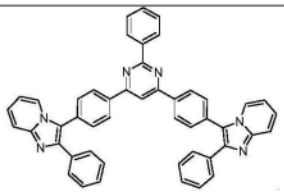	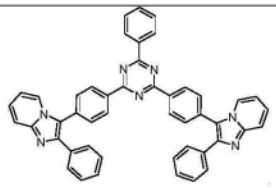
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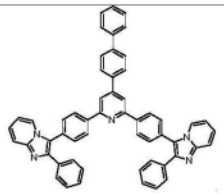	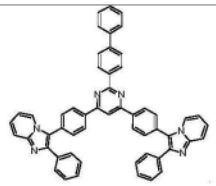	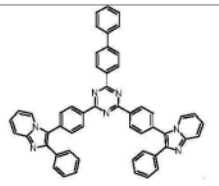
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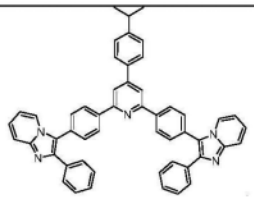	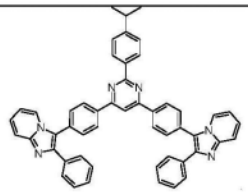	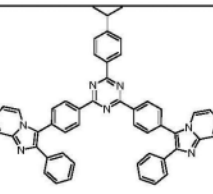
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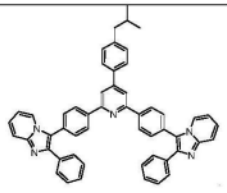	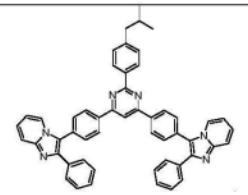	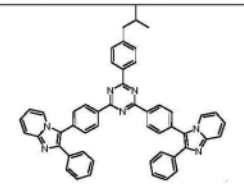
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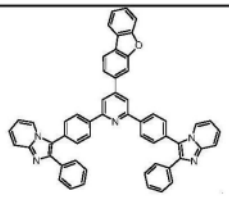	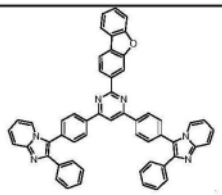	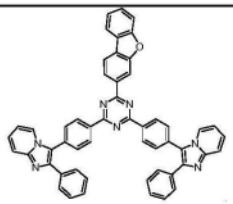
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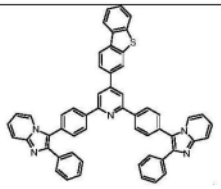	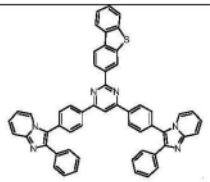	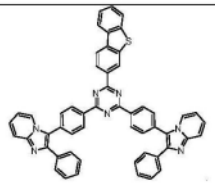
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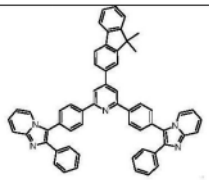	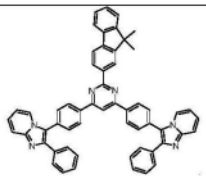	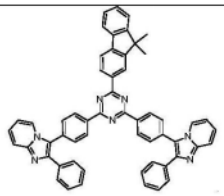
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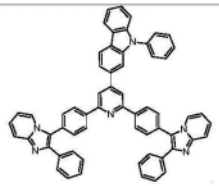	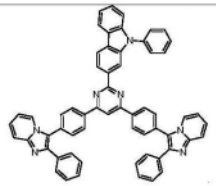	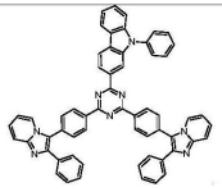
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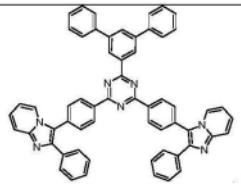	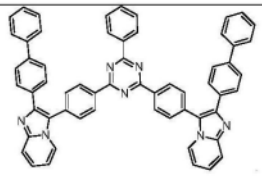	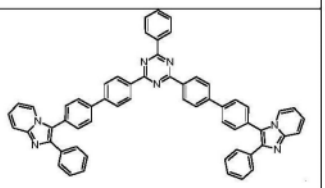
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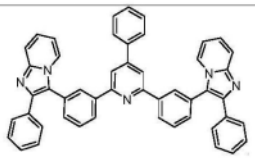	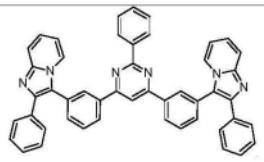	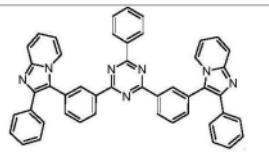
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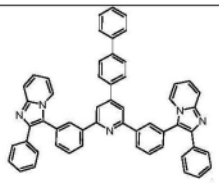	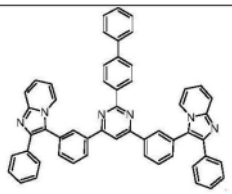	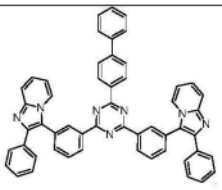

[0027]

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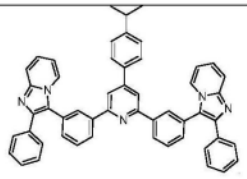	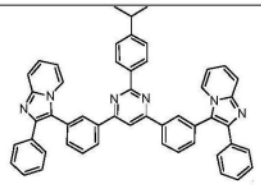	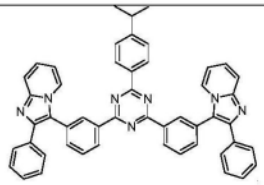
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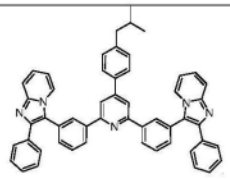	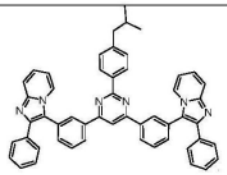	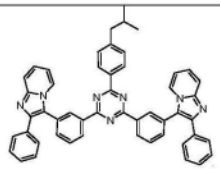
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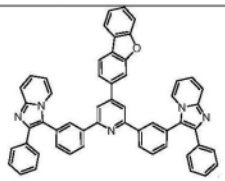	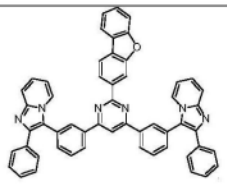	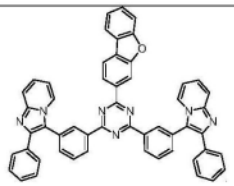
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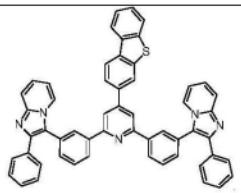	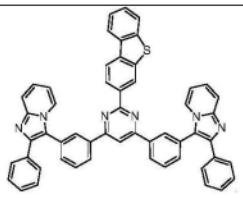	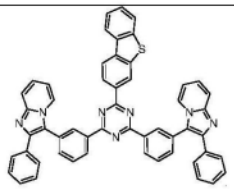
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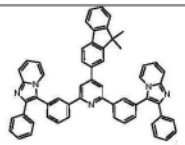	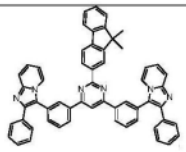	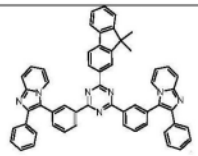
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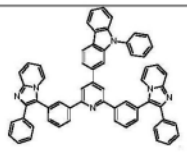	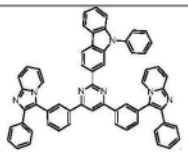	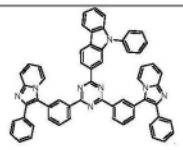
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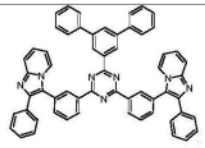
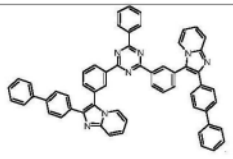
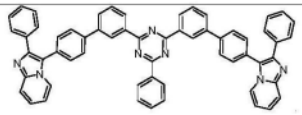
		

[0028] 优选:式(I)所述化合物,其中X1、X2、X3表示为CH。

[0029] 进一步优选:其中R_1为单键、C1-C30烷基取代或未取代的C6-C30的非稠环芳基、C1-C30烷基取代或未取代的C3-C27的非稠环杂芳基;其中R_2为C1-C30烷基取代或未取代的

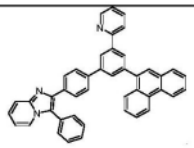
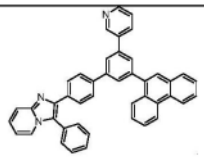
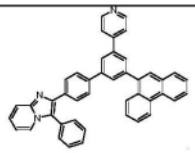
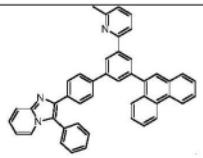
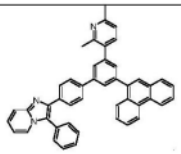
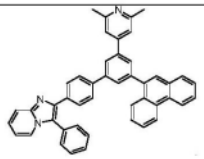
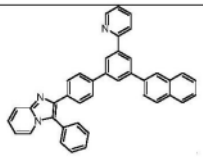
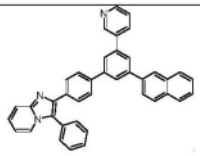
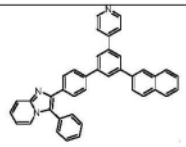
C6-C60的芳基、C1-C30烷基取代或未取代的C1-C60的杂芳基;R3、R4为氢、氘、卤素、烷基、杂烷基、环烷基、C1-C30烷基取代或未取代的C6-C60的芳基、C1-C30烷基取代或未取代的C1-C60的杂芳基、经取代或未经取代的单环或多环C3-C60脂肪族环或芳香族环且R3、R4中至少有一个为C1-C30烷基取代或未取代的C6-C60的芳基、C1-C30烷基取代或未取代的C1-C60的杂芳基、经取代或未经取代的单环或多环C3-C60脂肪族环或芳香族环。

[0030] 再优选:其中R1为单键、C1-C4烷基取代或未取代的C6-C18的非稠环芳基、C1-C4烷基取代或未取代的C3-C15的非稠环杂芳基;R2为C1-C4烷基取代或未取代的C6-C18的芳基、C1-C4烷基取代或未取代的C3-C15的杂芳基;R3、R4为氢、氘、卤素、烷基、C1-C4烷基取代或未取代的C6-C18的芳基、C1-C4烷基取代或未取代的C3-C15的杂芳基、经取代或未经取代的单环或多环C3-C18脂肪族环或芳香族环且R3、R4不同。

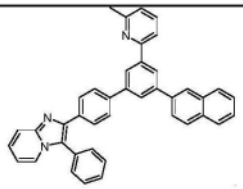
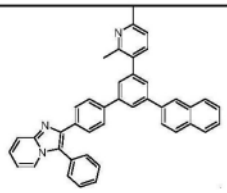
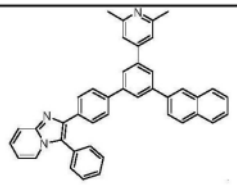
[0031] 更优选:其中R1为单键、C6-C18的非稠环芳基或C3-C15的非稠环杂芳基;R2为C6-C18的芳基或C3-C15的杂芳基。

[0032] 作为优选的化合物为以下化合物:

[0033]

B 1	B 2	B 3
		
B 4	B 5	B 6
		
B 7	B 8	B 9
		
B 10	B 11	B 12

[0034]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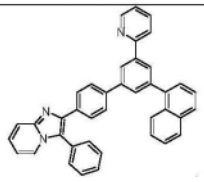
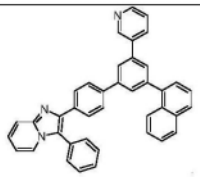
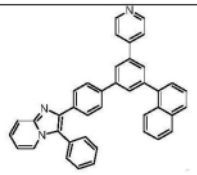
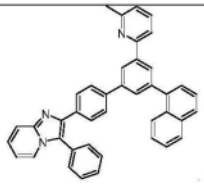
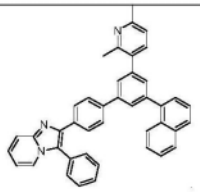
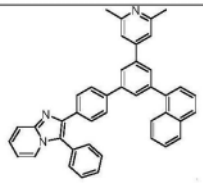
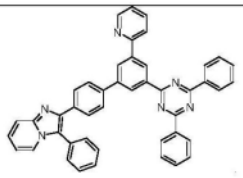
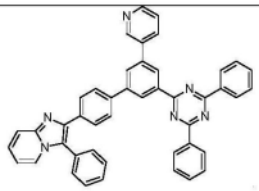
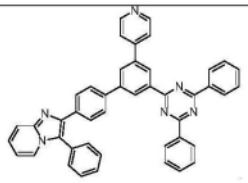
		
B 16	B 17	B 18
		
B 19	B 20	B 21
		
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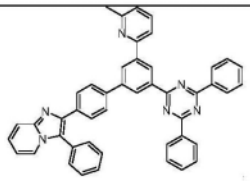	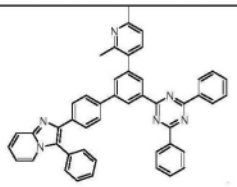	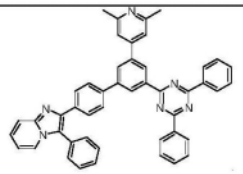
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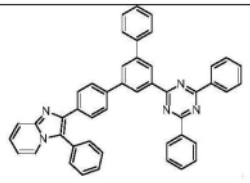	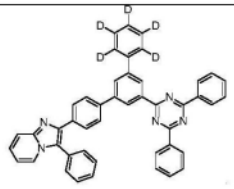	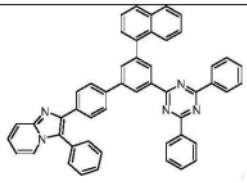
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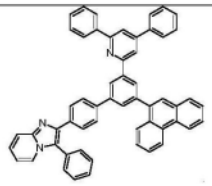	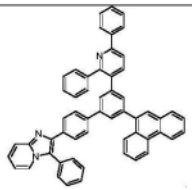	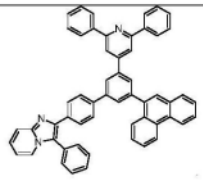

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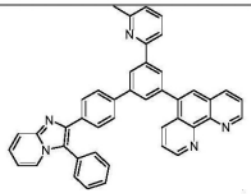	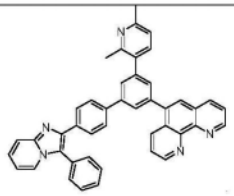	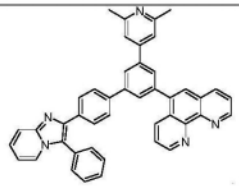
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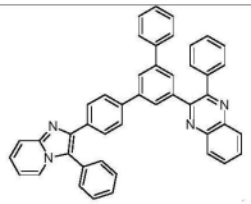	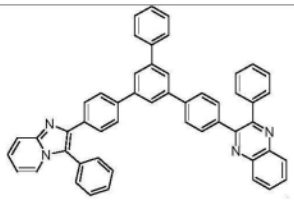	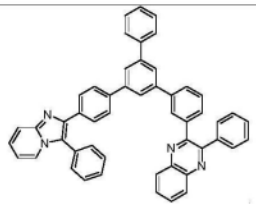
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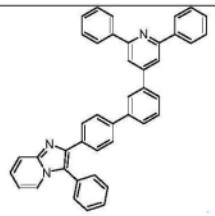	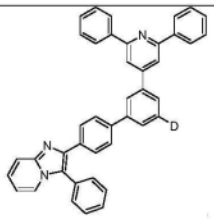	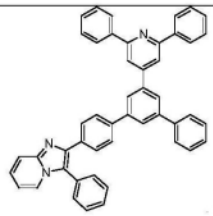
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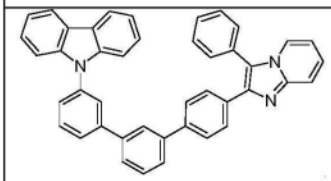	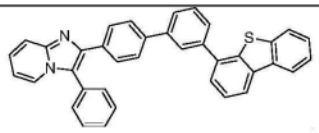	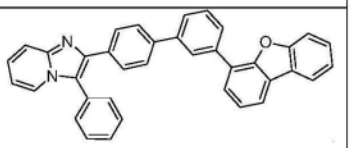
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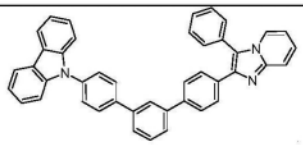	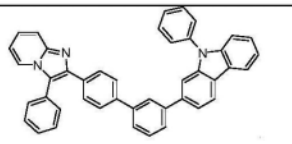	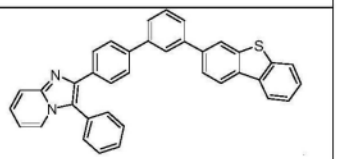
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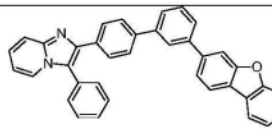
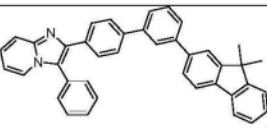
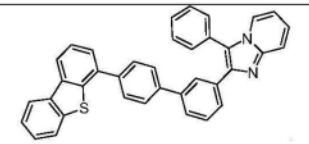
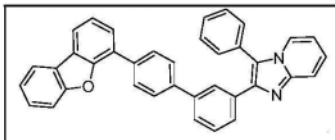
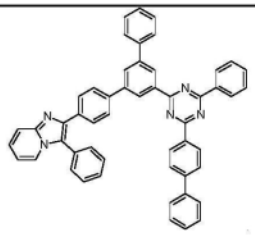
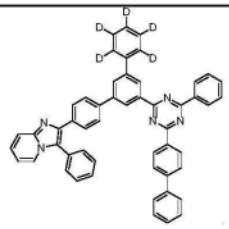
		
B 49	B 50	B 51

[0036]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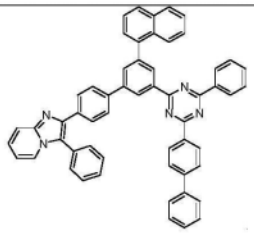	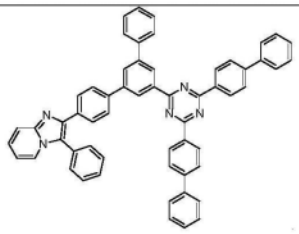	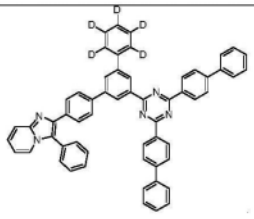
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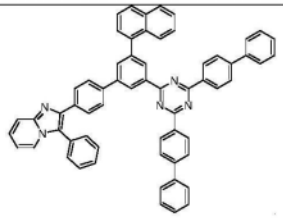	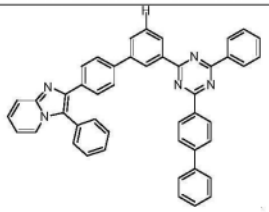	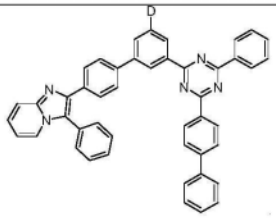
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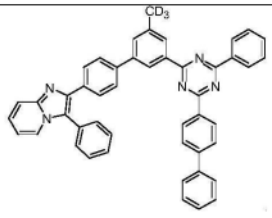	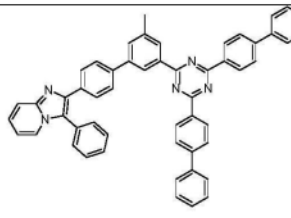	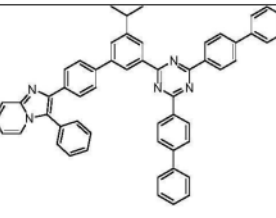
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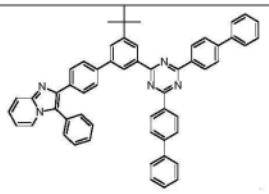	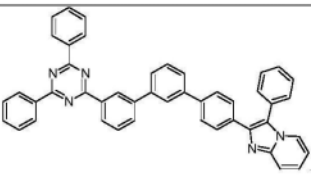	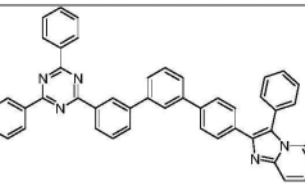
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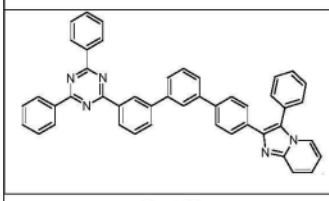
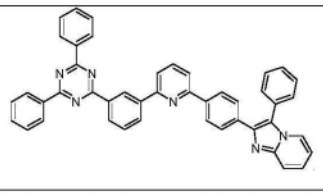
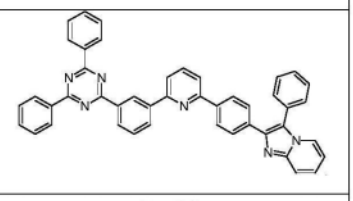
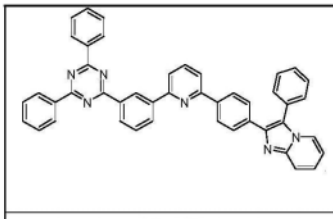
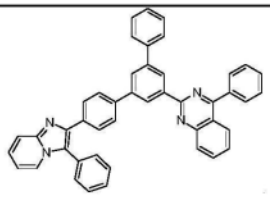
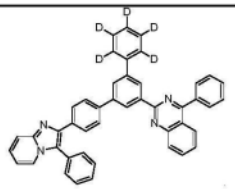
		
B 67	B 68	B 69

[0037]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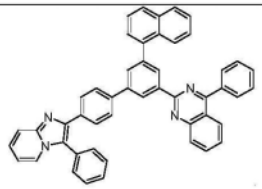	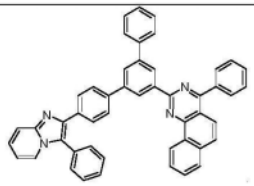	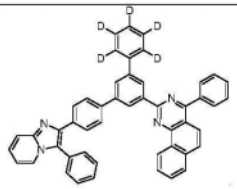
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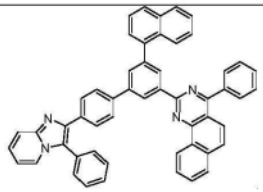	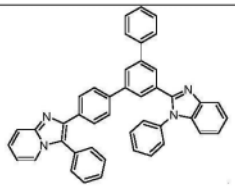	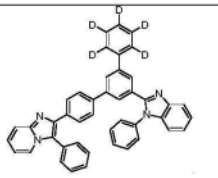
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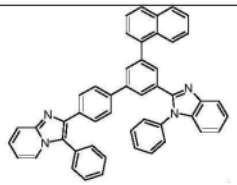	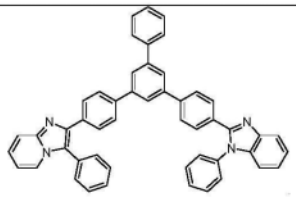	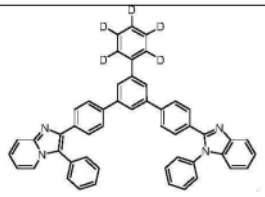
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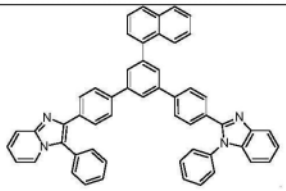	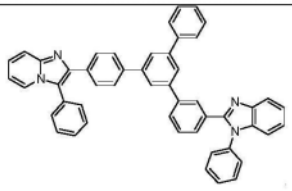	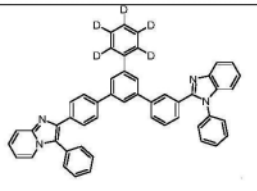
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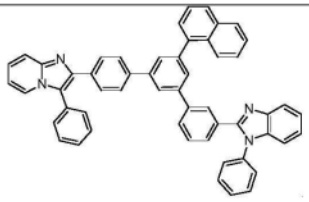	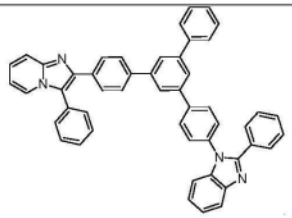	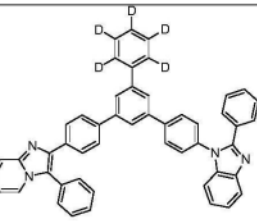
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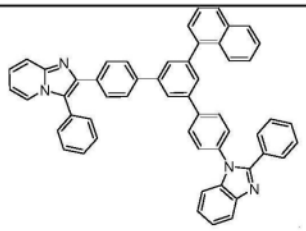
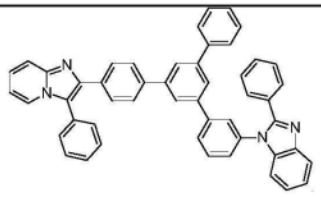
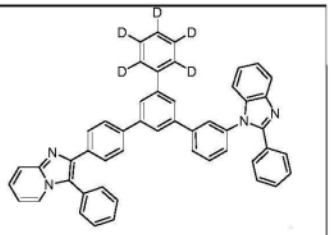
[0038]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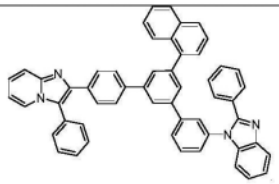	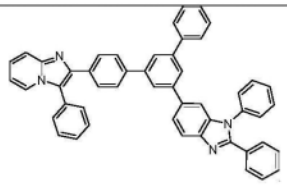	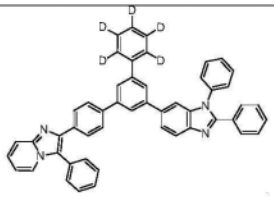
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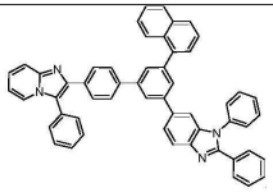	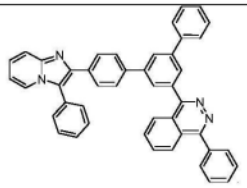	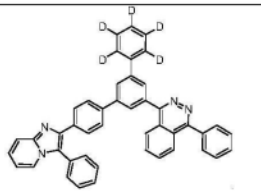
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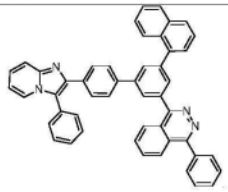	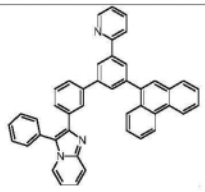	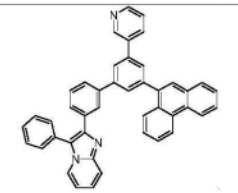
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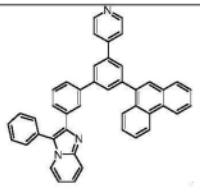	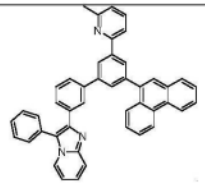	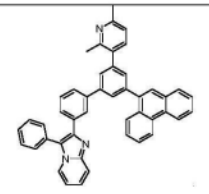
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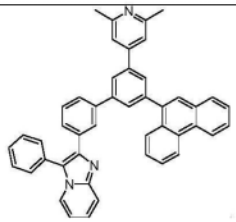	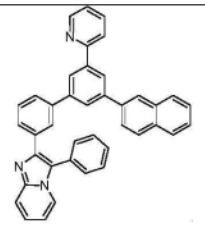	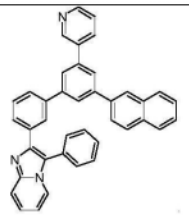
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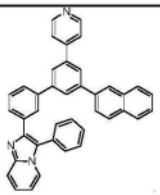
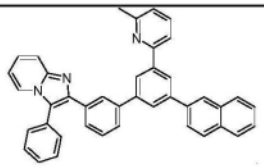
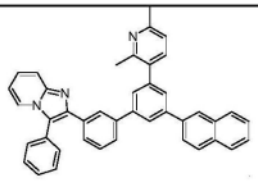
[0039]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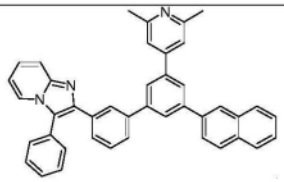	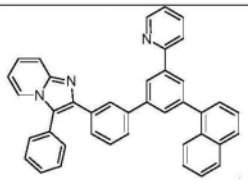	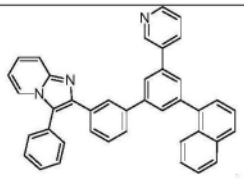
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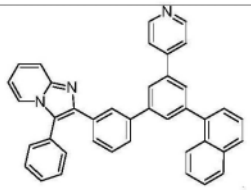	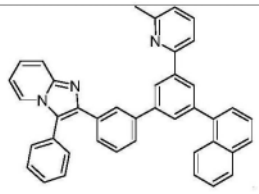	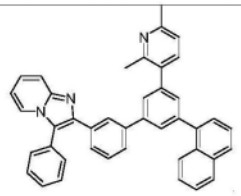
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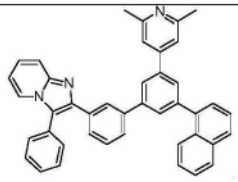	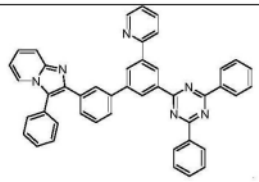	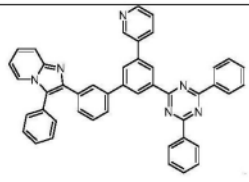
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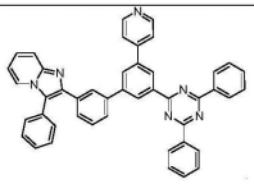	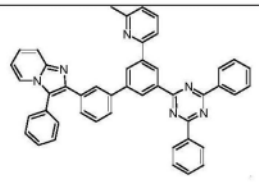	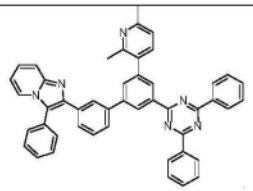
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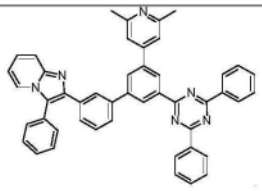	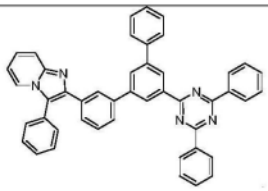	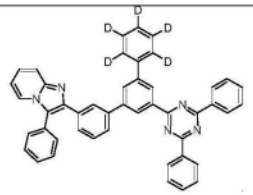
B 121	B 122	B 123

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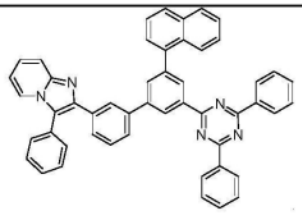	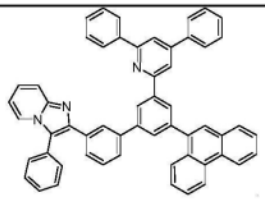	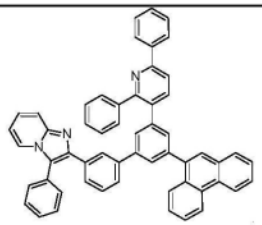
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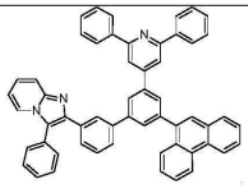	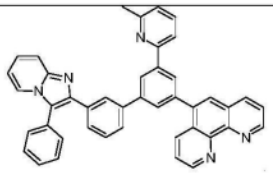	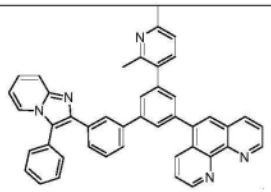
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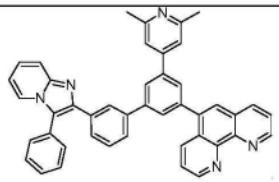	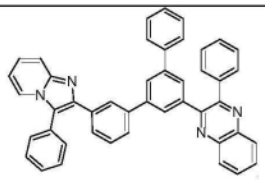	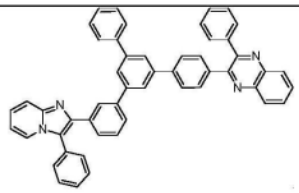
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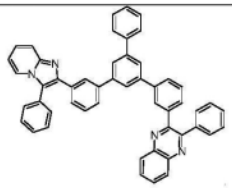	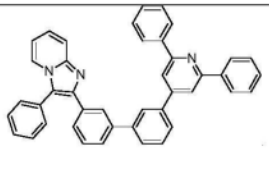	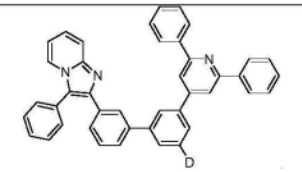
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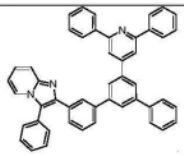	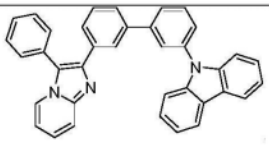	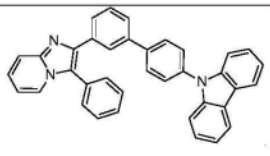
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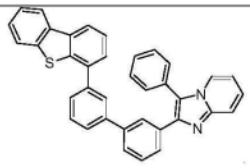	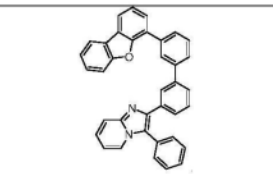	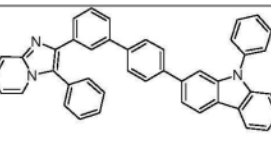
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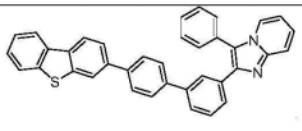	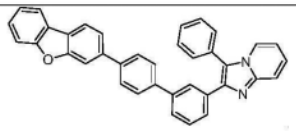	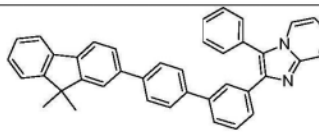
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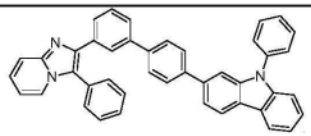	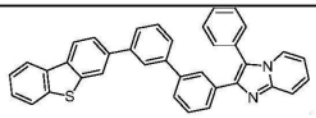	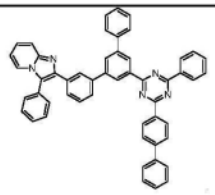
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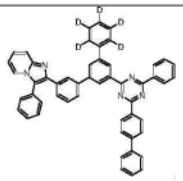	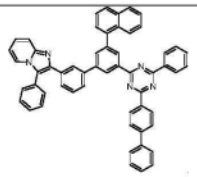	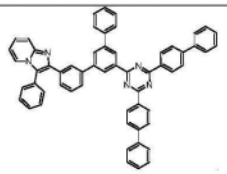
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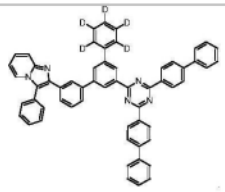	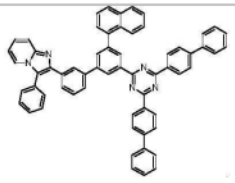	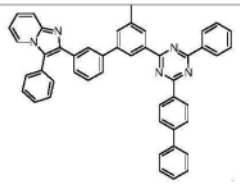
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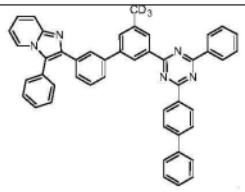	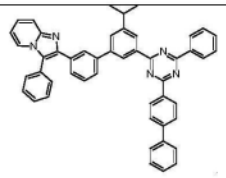	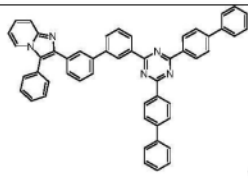
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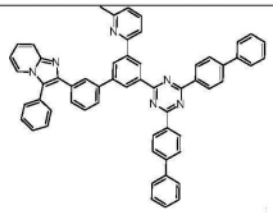	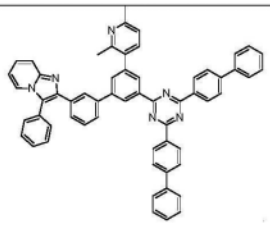	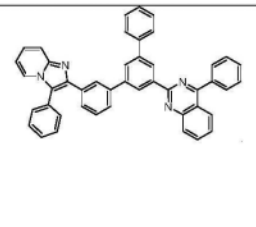
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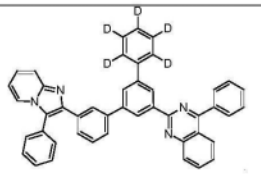	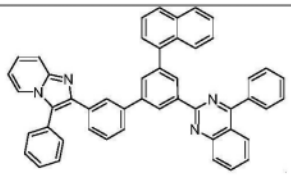	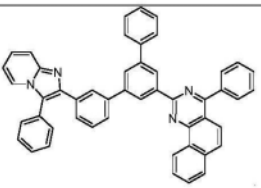
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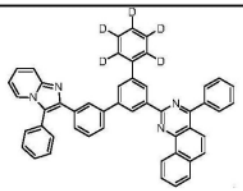
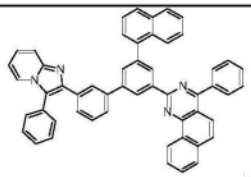
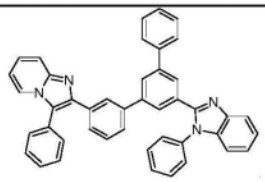
[0042]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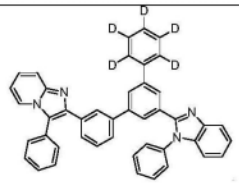	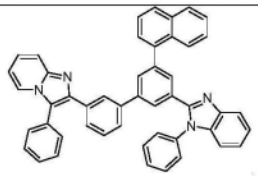	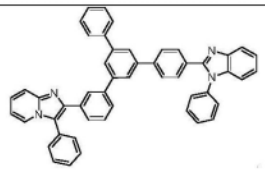
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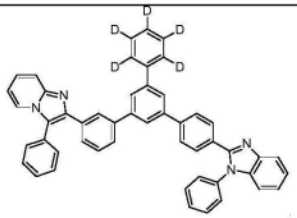	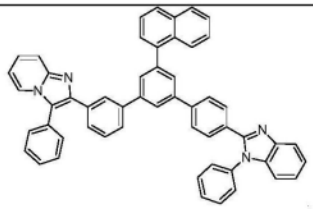	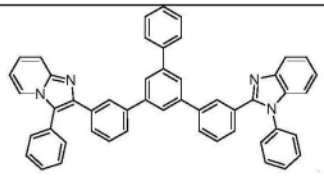
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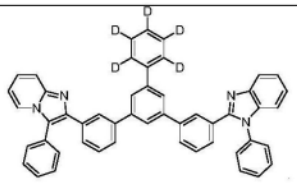	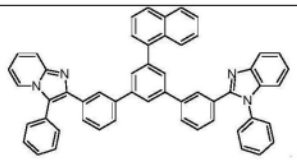	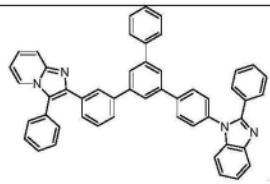
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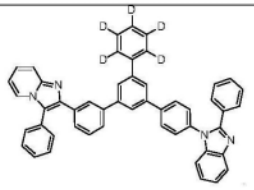	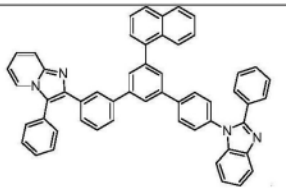	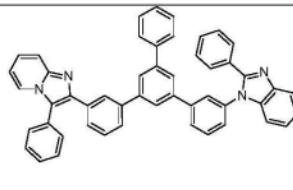
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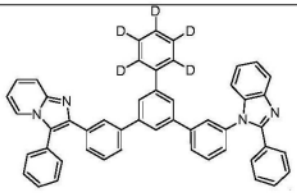
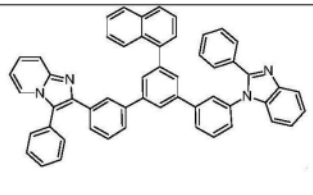
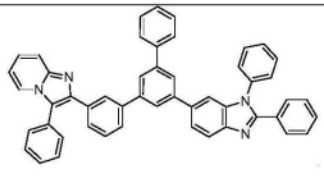
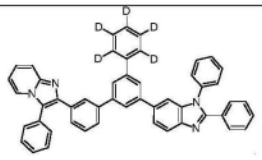
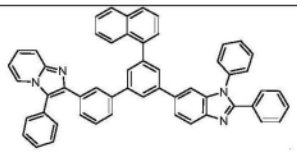
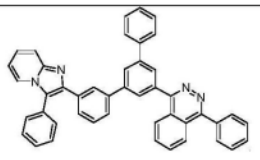
		
B 178	B 179	B 180
		

[0043]

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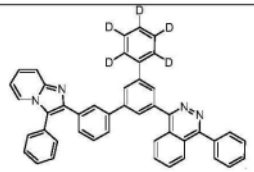
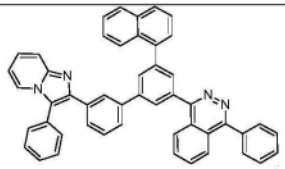
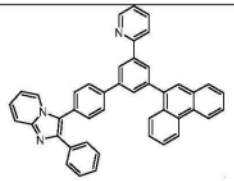
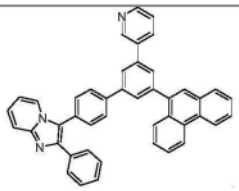
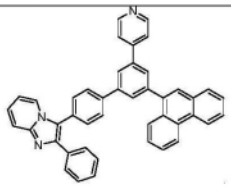
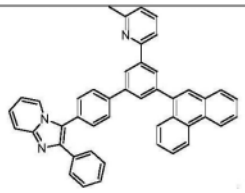
		
B 184	B 185	B 186
		
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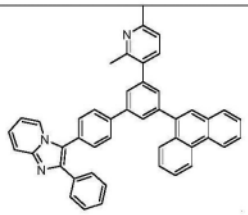	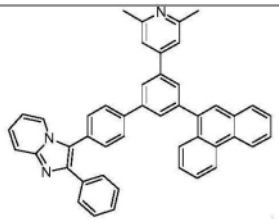	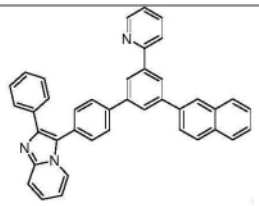
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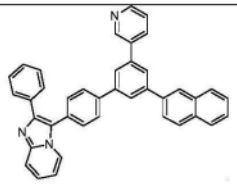	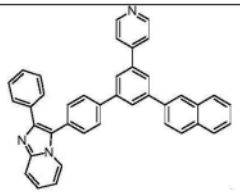	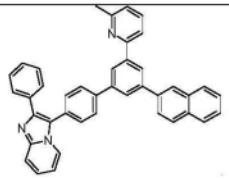
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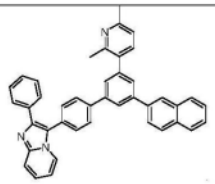	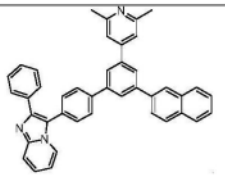	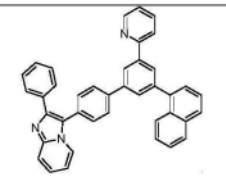
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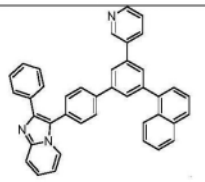	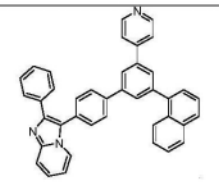	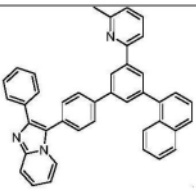
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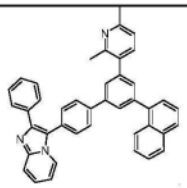	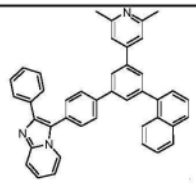	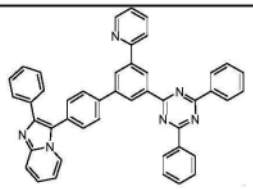
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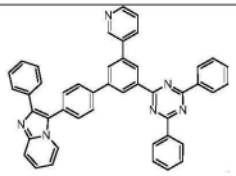	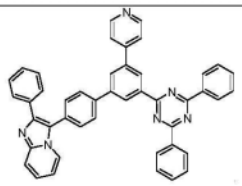	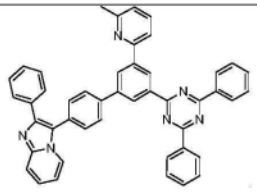
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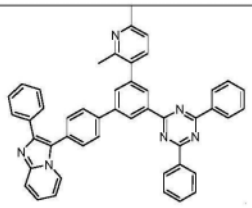	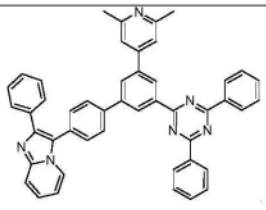	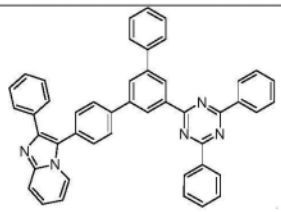
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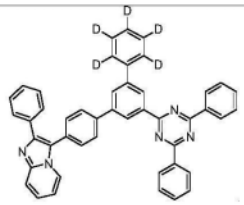	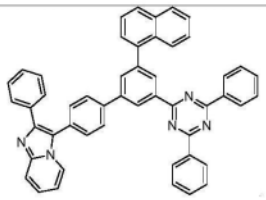	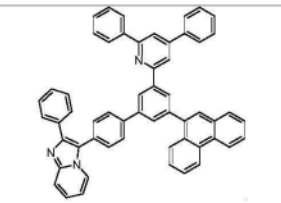
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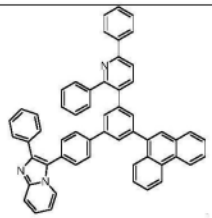	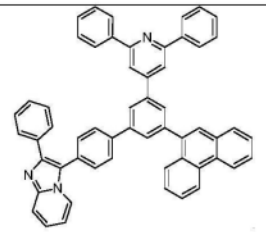	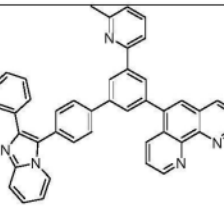
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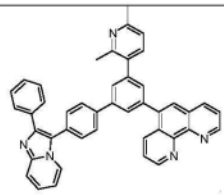	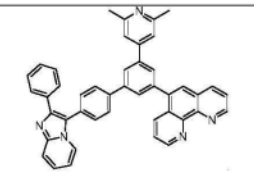	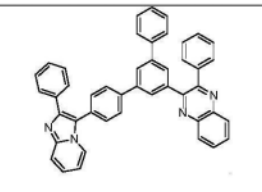
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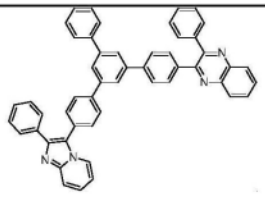	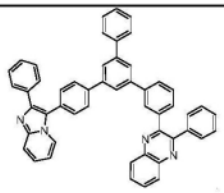	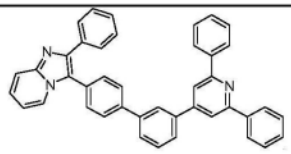
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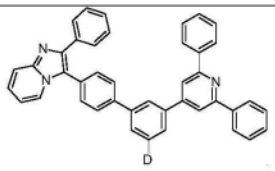	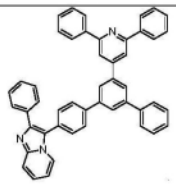	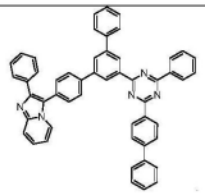
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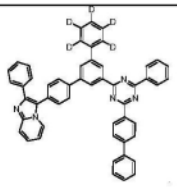	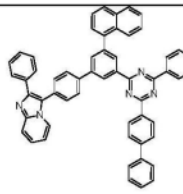	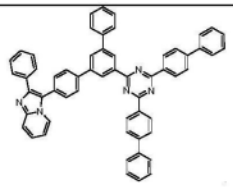
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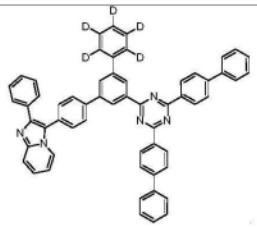	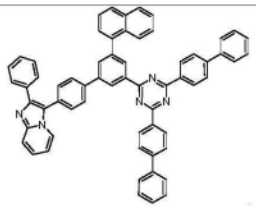	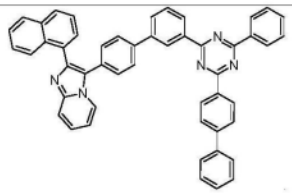
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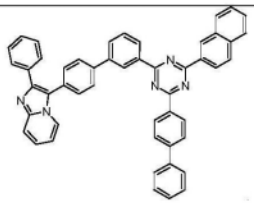	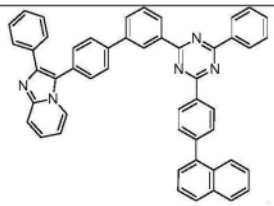	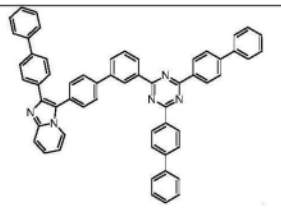
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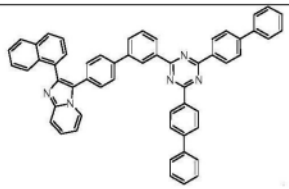	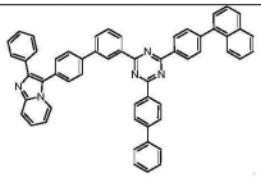	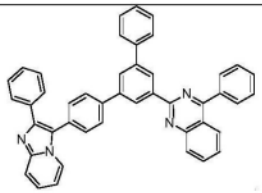
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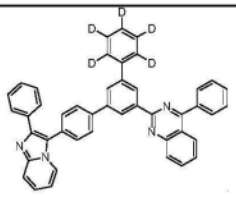	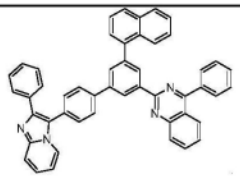	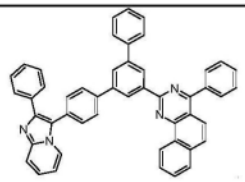
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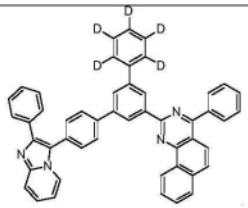	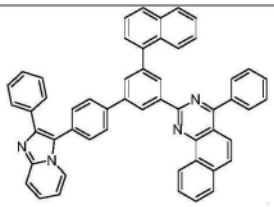	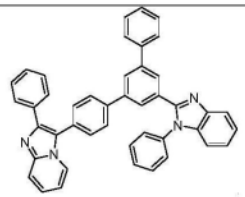
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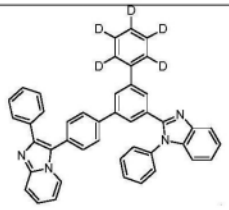	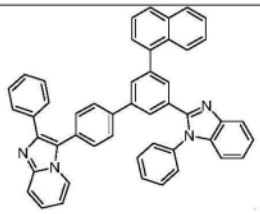	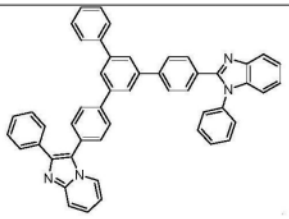
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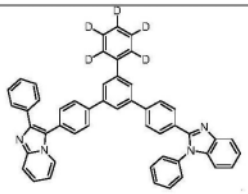	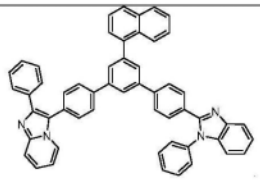	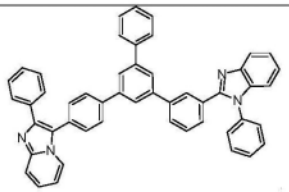
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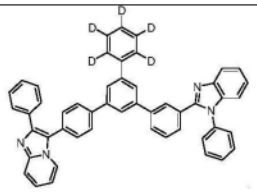	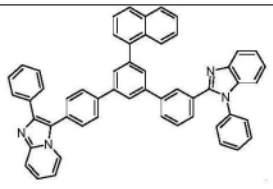	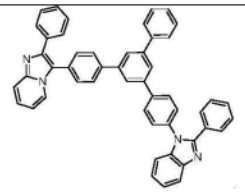
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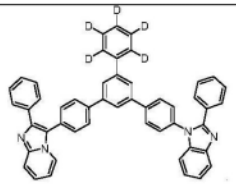	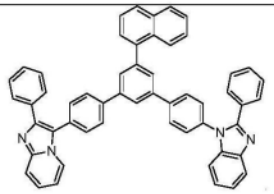	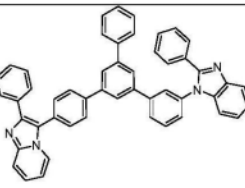
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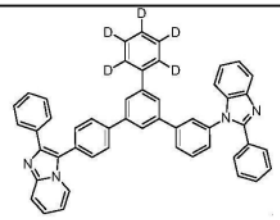	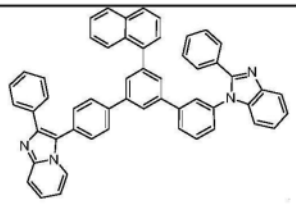	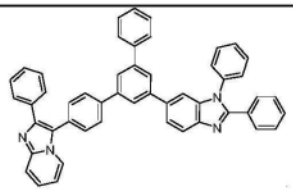
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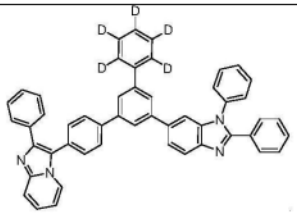	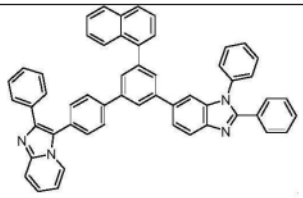	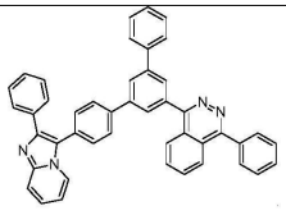
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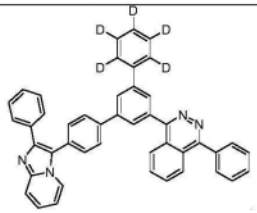	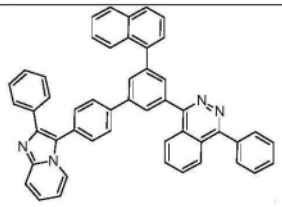	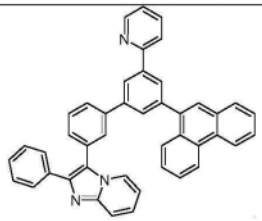
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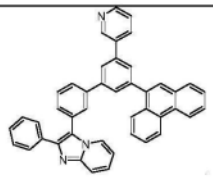	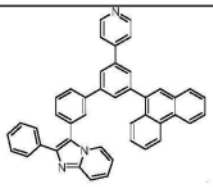	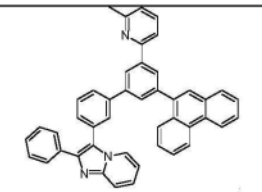
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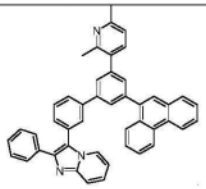	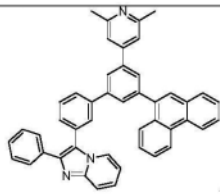	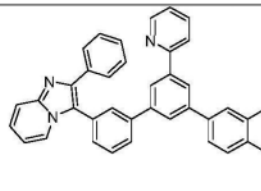
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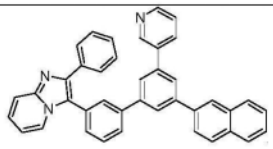	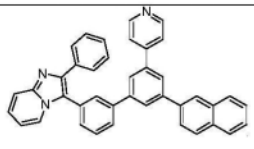	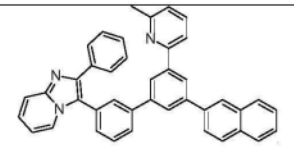
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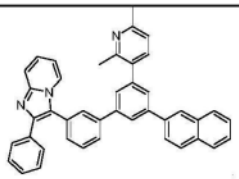	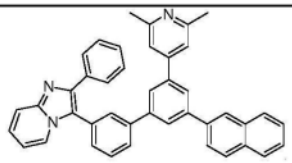	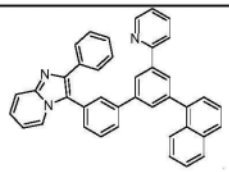
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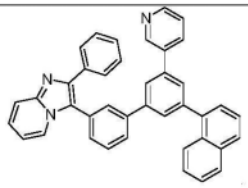	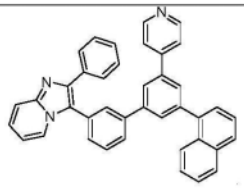	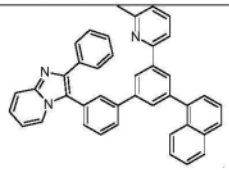
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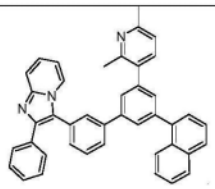	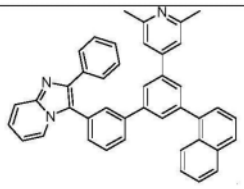	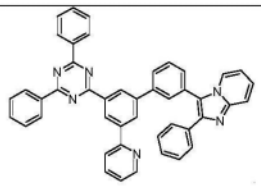
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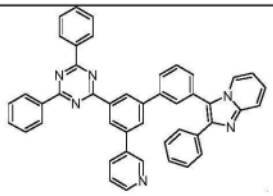	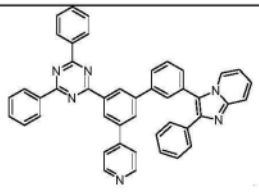	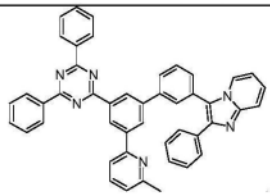
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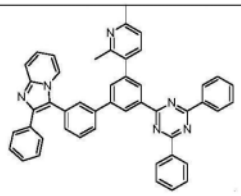	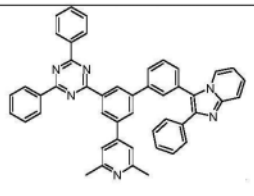	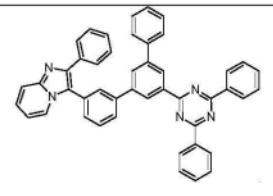
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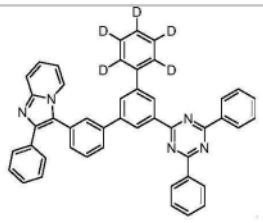	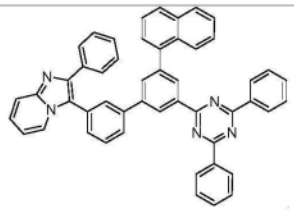	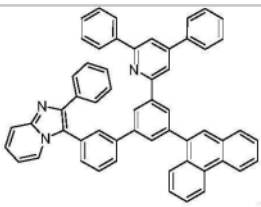
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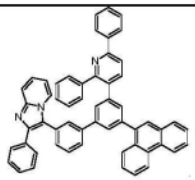	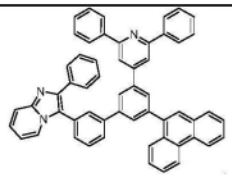	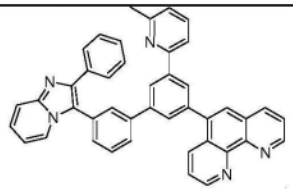
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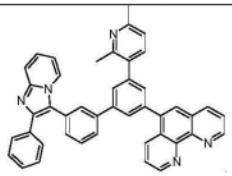	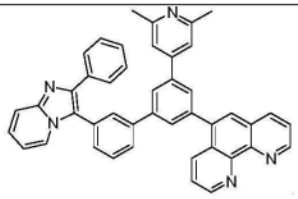	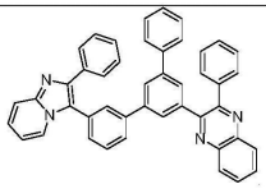
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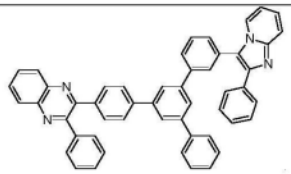	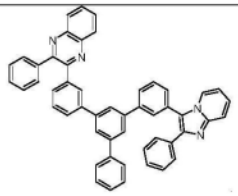	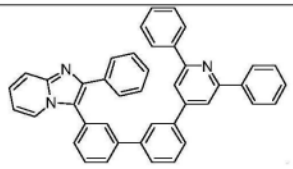
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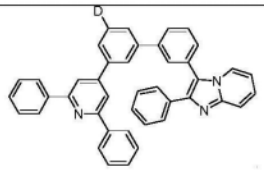	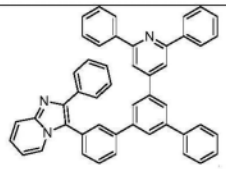	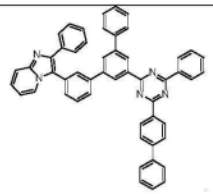
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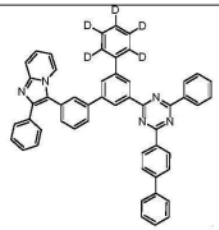	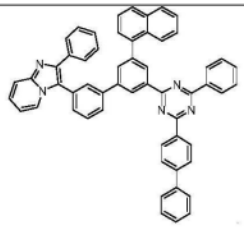	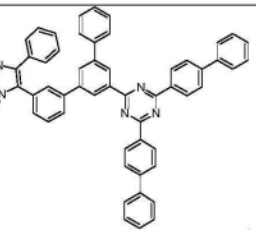
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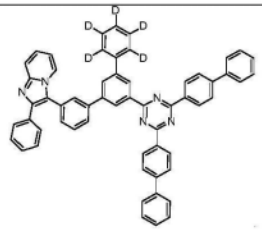
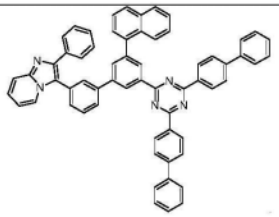
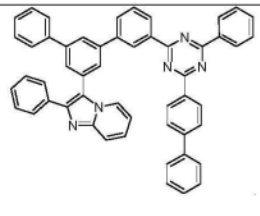
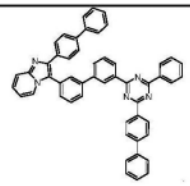
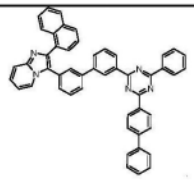
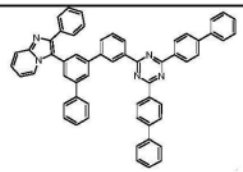
		
B 307	B 308	B 309

[0050]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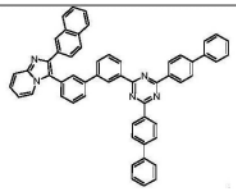	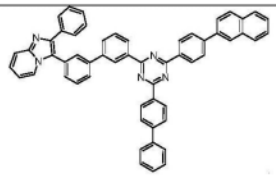	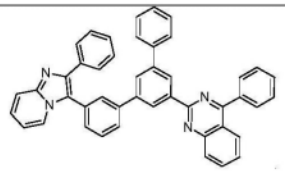
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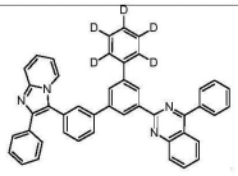	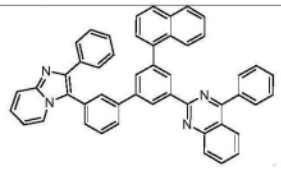	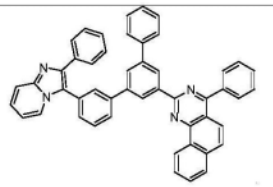
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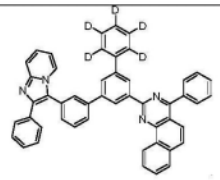
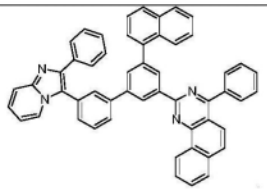
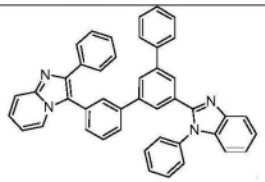
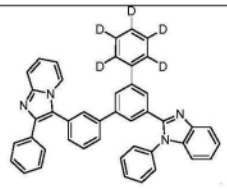
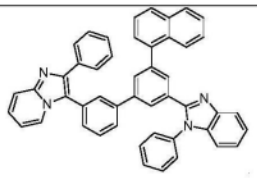
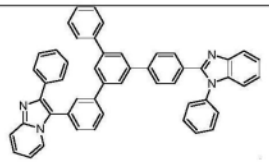
		
B 319	B 320	B 321
		
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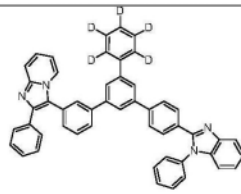
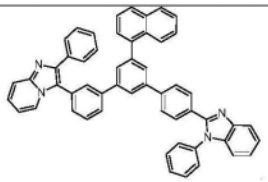
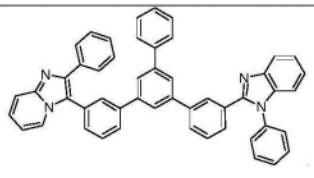
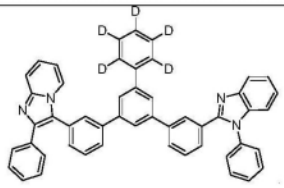
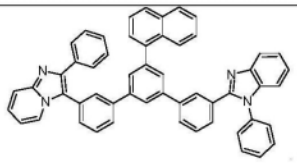
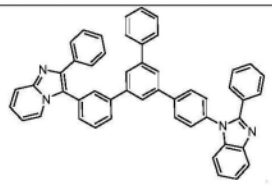
		
B 325	B 326	B 327
		

[0051]

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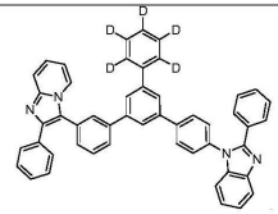	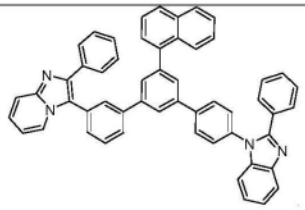	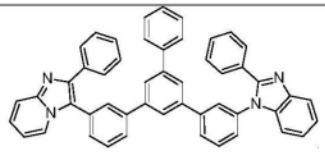
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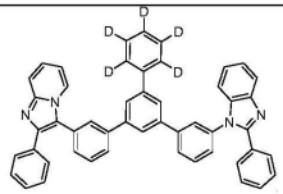	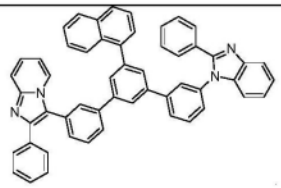	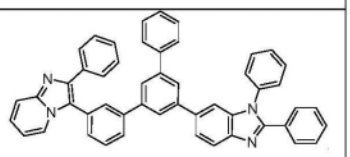
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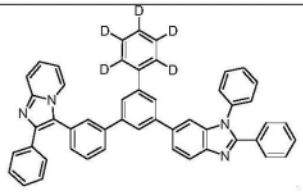
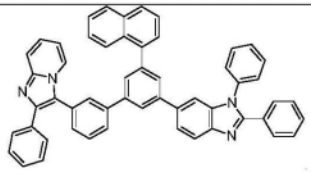
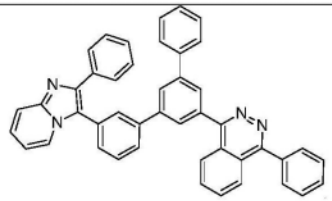
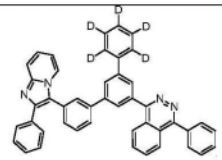
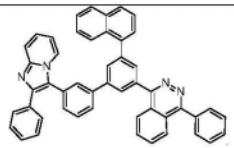
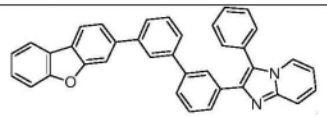
		
B 337	B 338	B 339
		
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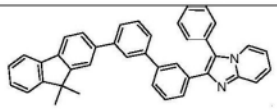
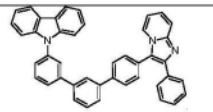
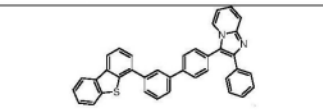
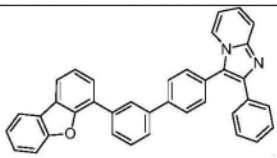
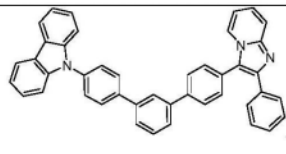
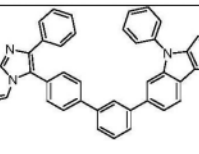
		
B 343	B 344	B 345
		
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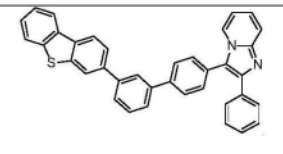	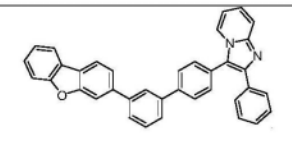	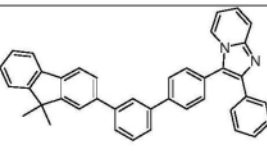
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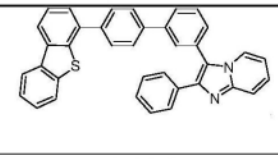
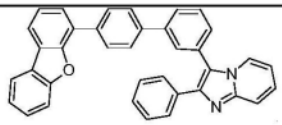
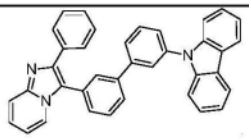
[0052]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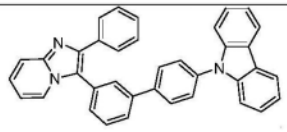	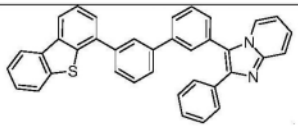	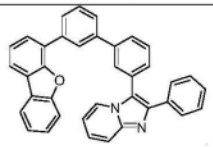
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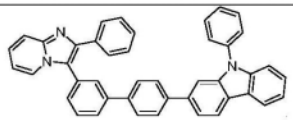	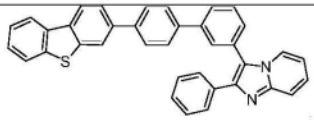	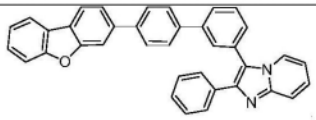
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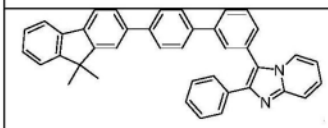	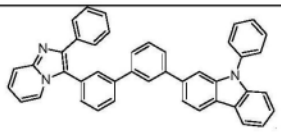	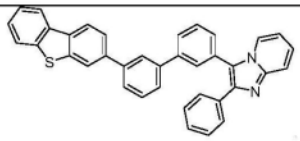
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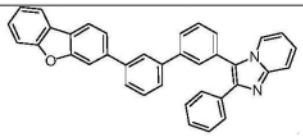
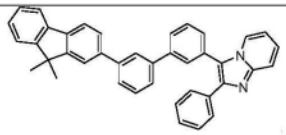
		

[0053] 上述化合物在OLED器件中的应用。

[0054] 所述应用为化合物作为OLED器件的电子传输层材料、空穴阻隔层材料和/或光提取层材料。

[0055] 本发明的化合物材料具有升华温度低,光、电、热稳定性好,发光效率高,电压低、寿命长,折射率高、可见光区折射率差异小等优点,可用于有机发光器件中,特别是作为电子传输材料、空穴阻隔层材料、光提取层材料,该器件具有驱动电压低、发光效率高、器件寿命长的优点,具有应用于AMOLED产业的可能。

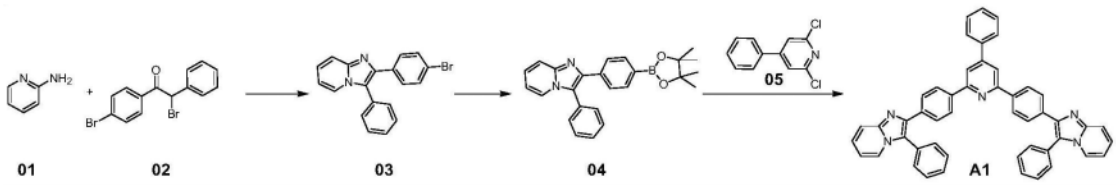
[0056] 具体实施方式(合成和器件实施):

[0057] 下述实施例仅仅是为了便于理解技术发明,不应视为本发明的具体限制。

[0058] 本发明中的化合物合成中涉及的原物料和溶剂等均购自于Alfa、Acros等本领域技术人员熟知的供应商。

实施例:

[0059] (1)化合物A1的合成:

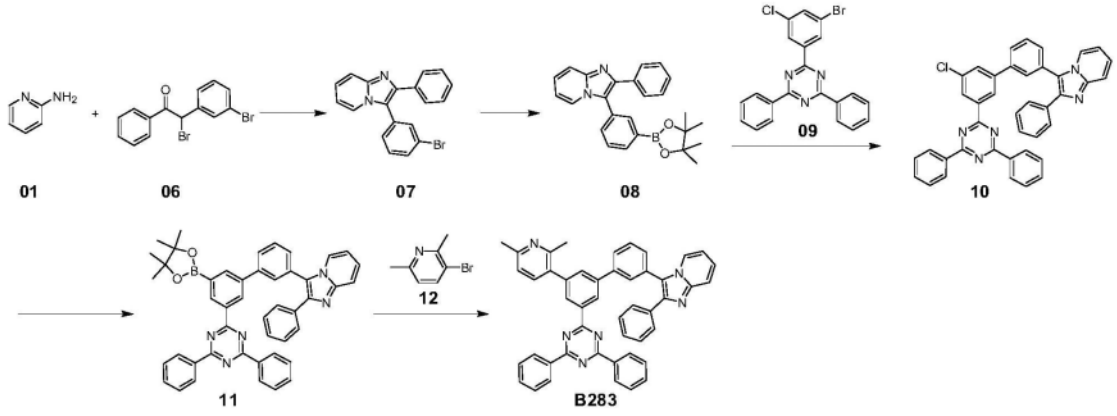
[0060] 

[0061] 化合物03的合成:向一个2L单口瓶,依次将化合物01(53.17g,0.57mol,1.0eq)、化合物02(200g,0.57mol,1.0eq),NaHCO3(94.9g,1.14mol,2.0eq)、异丙醇(1000ml)投入到烧瓶中,油浴加热到80度左右,保温搅拌回流7h,取样点板原料反应完。降温,滴加去离子水,搅拌4h左右,抽滤。固体用乙醇打浆,抽滤烘干。得到157g白色固体化合物03,收率79.6%。质谱:349.03(M+H)

[0062] 化合物04的合成:向一个1L单口瓶,依次加入化合物03(60g,171.81mmol,1.0eq)、双联频呐硼酸酯(56.72g,223.35mmol,1.3eq)、Pd(dppf)Cl2(1.26g,1.72mmol,0.01eq)、CH3COOK(33.72g,343.62mmol,2.0eq),600ml二氧六环,搅拌下N2置换3次,加热,回流3h。TLC监测反应完全(EA/Hex=1:8)。反应液降至室温,真空浓缩二氧六环至无溶剂馏出,加入600mlDCM将固体溶解,用水200ml洗一次,将水相用200mlDCM提一次,合并有机相,并用水洗两次(每次200ml),将有机相有无水MgSO4干燥。过硅胶滤,并用DCM 300ml淋洗,浓缩有机相至仅剩150ml左右,加入正已烷500ml降至室温结晶2h。过滤,滤饼用正已烷100ml,淋洗,抽干得到59g,真空干燥过夜,得到54g类白色固体化合物04,收率78.2%。质谱:397.30(M+H)

[0063] 化合物A1的合成:向一个1L单口瓶,依次加入化合物04(45.06g,113.73mmol,2.1eq)、化合物05(12.62g,54.16mmol,1.0eq),Pd132(383.5mg,0.5416mmol,0.01eq),K_2CO_3(15.69g,113.73mmol,2.1eq),甲苯450ml,乙醇150ml,水150ml搅拌下N2置换3次,加热,回流20h。TLC监测反应完全,。降至室温后过滤,滤饼分别依次用水200ml,甲醇100ml,甲苯100ml,甲醇100ml淋洗,抽干,得到灰白色固体37g。将所得固体用THF重结晶,得到28g白色固体化合物A1。得到的化合物经过升华纯化得到21克米白色固体化合物A1,收率75%。质谱:692.28(M+H);1H NMR(400MHz,CDCl3)δ8.13(d,J=8.4Hz,4H),7.98(d,J=6.9Hz,2H),7.87(s,2H),7.81(d,J=8.3Hz,4H),7.72(t,J=8.4Hz,4H),7.58-7.43(m,13H),7.24-7.19(m,2H),6.75(t,J=6.8Hz,2H)。

[0064] (2)化合物B283的合成:

[0065] 

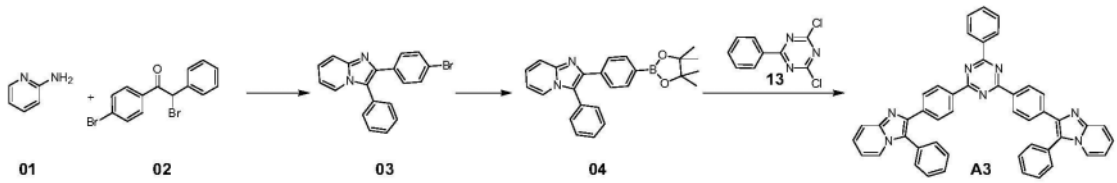
[0066] 化合物08的合成:参照化合物A1合成过程中,化合物04的合成方式和处理方法,只需要将对应的原物料变更即可。质谱:397.30(M+H);

[0067] 化合物10的合成:将化合物08(22g,55.53mmol,2.1eq)、化合物09(22.5g,53.44mmol,1.04eq)、K_2CO_3(11g,79.71mmol,1.5eq)、$Pd(PPh_3)_4$(1.2g,1.04mmol,0.02eq)、甲苯(400ml)、乙醇(50ml)、水(50ml)依次加入到1L的四口烧瓶中,置换N2三次,升温至80℃,搅拌6小时,TLC显示反应完全。反应液降温后,过滤,滤渣用乙醇/水打浆,抽滤得25g灰色固体化合物10,收率75%。质谱:612.19(M+H);

[0068] 化合物11的合成:将化合物10(25g,40.90mmol,1.0eq)、双联频呐硼酸酯(15.5g,61mmol,1.5eq)、X-Phos(0.8g,1.68mmol,0.04eq)、CH_3COOK(8g,81.52mmol,2.0eq)、dioxane(400ml)、$Pd(OAc)_2$(183mg,0.81mmol,0.02eq)依次加入至1L的四口烧瓶中,置换N2三次,升温至105℃,搅拌3小时,TLC显示反应完全。反应液降温后,加DCM(200ml),硅胶过滤,母液水洗后旋干,得到的残渣用甲苯/正己烷重结晶得26g白色固体化合物11,收率91%。质谱:704.31(M+H);

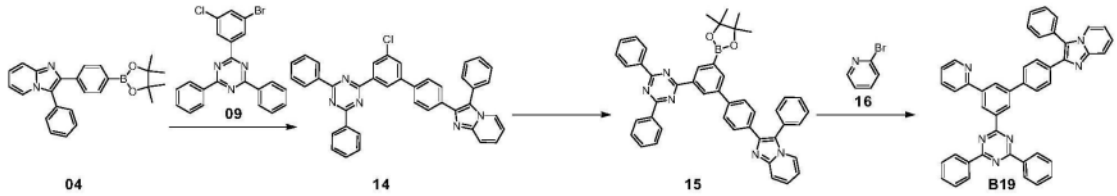
[0069] 化合物B283的合成:将化合物11(26g,36.97mmol,1.0eq)、化合物12(10.3g,55.67mmol,1.5eq)、K_2CO_3(10.2g,73.91mmol,2.0eq)、Pd-132(0.5g,0.7061mmol,0.02eq)、甲苯(300ml)、乙醇(50ml)、水(50ml)依次加入至1L的四口烧瓶中,置换N2三次,开始升温体系至85℃,搅拌5小时,反应完全。降温后反应液加DCM稀释(500ml),滤硅胶,母液水洗后旋干得25g粗品,残渣用Tol/hex重结晶得12g白色固体化合物B283,收率48%。得到的化合物经过升华纯化得到7.56克米白色固体化合物B283,收率63%。质谱:683.28(M+H);1H NMR(400MHz,CDCl3)δ8.99(s,1H),8.77-8.73(m,5H),8.13-8.11(d,2H),7.99-7.87(m,2H),7.78-7.69(m,5H),7.64-7.52(m,8H),7.34-7.29(t,2H),7.24-7.21(t,2H),7.14-7.12(d,1H),2.64(s,3H),2.60(s,3H)。

[0070] (3)化合物A3的合成:

[0071] 

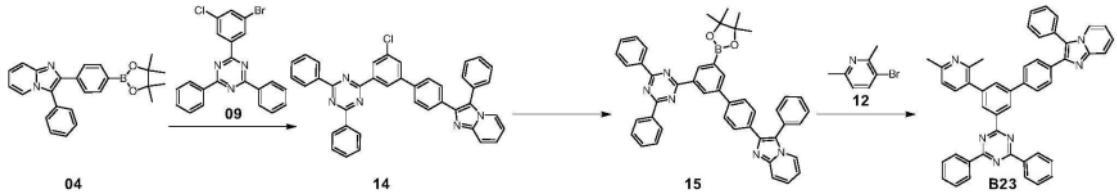
[0072] 化合物A3的合成:选取对应的材料,参照化合物A1的合成、升华得到黄色固体化合物A3。

[0073] (4)化合物B19的合成:

[0074] 

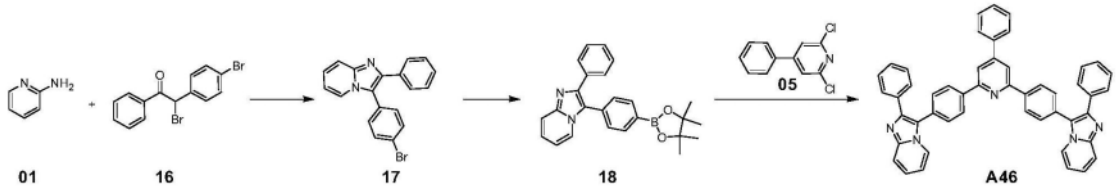
[0075] 化合物B19的合成:选取对应的材料,参照化合物B283的合成、升华得到米白色固体化合物B19。

[0076] (5)化合物B23的合成:

[0077] 

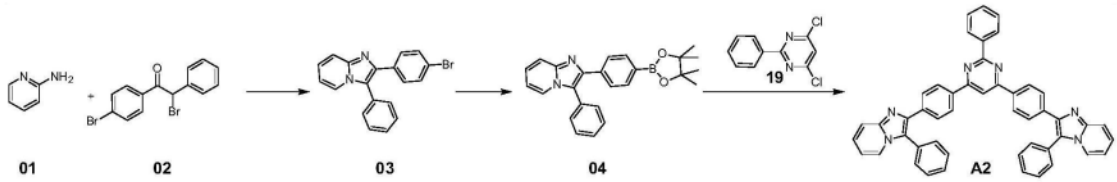
[0078] 化合物B23的合成:选取对应的材料,参照化合物B283的合成、升华得到米白色固体化合物B23。

[0079] (6)化合物A46的合成:

[0080] 

[0081] 化合物A46的合成:选取对应的材料,参照化合物A1的合成、升华得到黄色固体化合物A46。

[0082] (7)化合物A2的合成:

[0083] 

[0084] 化合物A2的合成:选取对应的材料,参照化合物A1的合成、升华得到黄色固体化合物A2。

[0085] 选取对应的材料,用同样类似的方法可以用于合成、升华得到其他化合物。

[0086] 应用例:

[0087] (1)化合物性能对比:本发明的化合物在OLED器件中可作为光提取层材料,具有较高的玻璃化转变温度、较高的折射率、可见光区较小的折射率差值。基本性能列于下表1

[0088] 表1:折射率对比:

[0089]

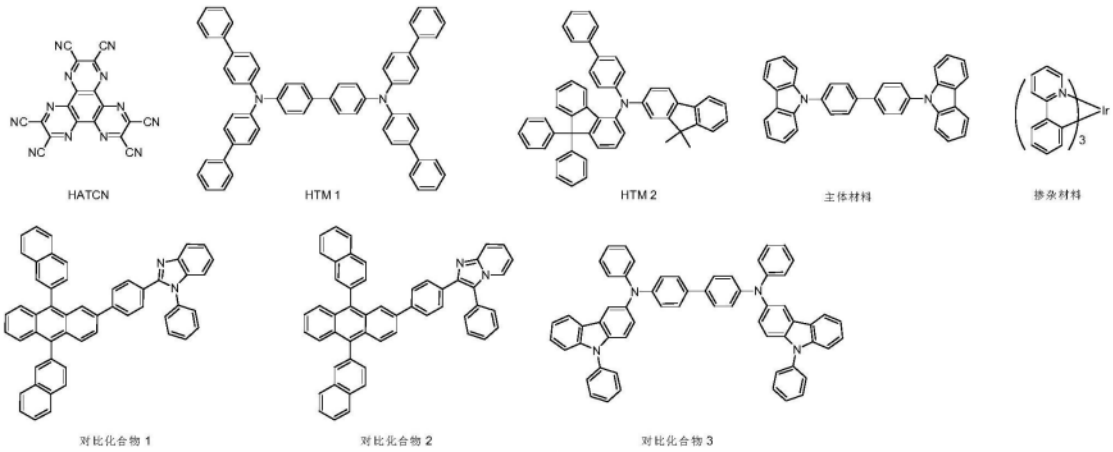
	玻璃化温度	折射率			折射率差值		
		@450nm	@520nm	@630nm	ΔB-G	ΔB-R	ΔG-R
化合物 **A1**	150	2.14	2.05	2.00	0.09	0.14	0.05
化合物 **B283**	128	2.02	1.96	1.94	0.06	0.08	0.02
化合物 **A3**	156	2.21	2.16	2.06	0.05	0.15	0.1
化合物 **B19**	134	2.09	2.03	1.98	0.06	0.11	0.05
化合物 **B23**	133	2.06	1.99	1.94	0.07	0.12	0.05
化合物 **A46**	158	2.03	1.95	1.91	0.08	0.12	0.04
化合物 **A2**	155	2.24	2.12	2.06	0.12	0.18	0.06
HTM1	134	1.99	1.91	1.85	0.08	0.14	0.06
对比化合物 3	132	1.99	1.89	1.84	0.1	0.15	0.05

[0090] (2)有机电致发光器件的制作

[0091] 将50mm*50mm*1.0mm的具有ITO(100nm)透明电极的玻璃基板在乙醇中超声清洗10分钟,再150度烘干后经过N2Plasma处理30分钟。将洗涤后的玻璃基板安装在真空蒸镀装置的基板支架上,首先在有透明电极线一侧的面上按照覆盖透明电极的方式蒸镀化合物HATCN,形成膜厚为5nm的薄膜,紧接着蒸镀一层HTM1形成膜厚为60nm的薄膜,再在HTM1薄膜上蒸镀一层HTM2形成膜厚为10nm的薄膜,然后,在HTM2膜层上再采用共蒸镀的模式蒸镀主体材料CBP和掺杂材料,膜厚为30nm,主体材料和掺杂材料比例为90%:10%。在发光层上再依次按照下表的搭配蒸镀HBL(5nm)作为空穴阻隔层材料、ETL(30nm)作为电子传输材料,接

着在电子传输材料层之上蒸镀LiF(1nm)作为电子注入材料,接着再采用共蒸镀的模式蒸镀Mg/Ag(18nm,1:9)作为阴极材料,最后在阴极材料之上按照下表的搭配蒸镀CPL(50nm)作为光提取层材料。

[0092]



[0093] 器件性能评价

[0094] 将上述器件进行器件性能测试,在各实施例和比较例中,使用恒定电流电源(Keithley 2400),使用固定的电流密度流过发光元件,使用分光辐射俩都系(CS 2000)测试发光波谱。同时测定电压值以及测试亮度为初始亮度的90%的时间(LT90)。结果如下表2:

[0095] 表2:

[0096]

	HBL	ETL	CPL	启动电压 V @3000nits	电流效率 Cd/A @3000nits	LT90@ 3000nits
实施例 1	化合物 **A1**	化合物 **A1**	HTM1	4.6	61	186
实施例 2	化合物 **B283**	化合物 **B283**	HTM1	4.5	63	175
实施例 3	化合物 **A3**	化合物 **A3**	HTM1	4.6	64	192
实施例 4	化合物 **B19**	化合物 **B19**	HTM1	4.4	62	169
实施例 5	化合物 **B23**	化合物 **B23**	HTM1	4.3	63	173
实施例 6	化合物 **A46**	化合物 **A46**	HTM1	4.5	61	181
实施例 7	化合物 **A2**	化合物 **A2**	HTM1	4.5	60	156
实施例 8	化合物 **B340**	化合物 **B283**	化合物 **A3**	4.2	68	216
实施例 9	对比化合物 1	对比化合物 1	化合物 **A3**	4.7	53	96
实施例 10	对比化合物 2	对比化合物 2	化合物 **A3**	4.7	55	130
实施例 11	化合物 **B340**	化合物 **B23**	化合物 **A3**	4.6	69	256
实施例 12	化合物 **B340**	化合物 **B9**	化合物 **A2**	4.7	67	234
对比例 1	对比化合物 1	对比化合物 1	HTM1	5.2	48	92
对比例 2	对比化合物 2	对比化合物 2	HTM1	4.9	50	125

[0097] 由上面表格中的数据对比可知,使用本发明的化合物应用于有机电致发光器件作为空穴阻隔层或电子传输层或光提取层材料,相较于对比化合物在驱动电压、发光效率、器件寿命都表现出更加优越的性能。

[0098] 上述结果表明本发明的化合物具有升华温度低,光、电、热稳定性好,折射率高、可见光区折射率差异小等优点,该化合物制备的器件具有电压低、寿命长,发光效率高等优点,可用于有机发光器件中。特别是作为电子传输材料、空穴阻隔层材料、光提取层材料,具有应用于AMOLED产业的可能。