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(54) **ORGANIC LIGHT-EMITTING DIODE MATERIALS**

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C07D 417/04	(2006.01)
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C07D 487/04	(2006.01)

(52) **U.S. Cl.**

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(57) **ABSTRACT**

Described herin are molecules for use in organic light emitting diodes. Example molecules comprise at least one acceptor moiety A, at least one donor moiety D, and optionally one or more bridge moieties B. Each moiety A is covalently attached to either the moiety B or the moeity D, each moiety D is covalently attached to either the moeity B or the moeity A, and each B is covalently attached to at least one moiety A and at least one moiety D. Values and preferred values of moieties A, D and B are defined herein.

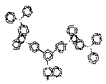
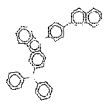
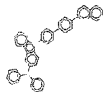
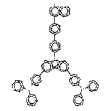
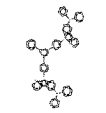
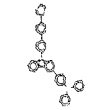
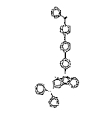
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november1-1	0.097	0.125	2.85	0.34	-4.96	-1.80	ZBLGYAMHOUKGJK	1039.4	3.8
		november2-2	0.150	0.081	2.65	0.02	-4.86	-1.92	OVVZYRCHMROADO	539.2	2.6
		november2-3	0.153	0.073	2.67	0.02	-4.84	-1.95	JYBUKVLNVAJWFK	615.2	2.8
		november3-4	0.040	0.057	2.69	1.16	-4.80	-1.91	AXEGAKOBNKIKOU	933.4	3.2
		november4-5	0.129	0.288	2.82	0.22	-4.87	-1.74	BBYZIFAMJLQQE	974.4	3.4
		november5-6	0.114	0.080	2.80	0.11	-4.80	-1.79	ILIJKARAJOZRMG	640.3	2.6
		november6-7	0.160	0.084	2.86	0.02	-4.91	-1.85	UZFJQNZNBHGSII	667.3	2.6

Table 1

FIGURE 1

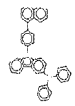
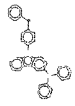
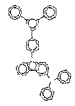
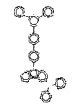
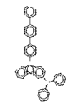
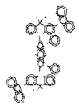
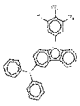
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november7-8	0.113	0.065	2.85	0.10	-4.94	-1.80	PDIYRWPDDXVUOQ	539.2	2.6
		november8-9	0.166	0.114	2.83	0.02	-4.90	-1.73	XPJCPLFUWIXGSI	515.2	2.4
		november9-10	0.138	0.165	2.72	0.09	-4.87	-1.84	JBKCTKNWQIVOFC	642.3	2.7
		november9-11	0.087	0.104	2.70	0.38	-4.84	-1.90	GMCPGGRZVQIYGJ	718.3	2.8
		november10-12	0.159	0.109	2.85	0.03	-4.91	-1.81	UBVBCCPDBALXBE	565.2	2.7
		november11-13	0.174	0.121	3.17	0.02	-5.14	-1.49	PBCQMQHRHRGLNX	1055.4	3.9
		november12-14	0.150	0.089	2.69	0.03	-5.14	-2.07	IGDGOLRVXRZJDF	615.1	3.0

FIGURE 2

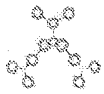
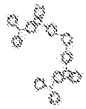
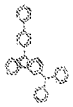
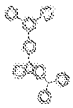
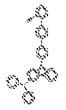
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november13-15	0.117	0.060	2.85	0.08	-4.81	-1.66	JIKPBZAYXYCJFJ	883.4	3.0
		november14-16	0.147	0.157	2.90	0.08	-4.87	-1.64	VMWHUNGZOULRR	897.4	3.2
		november14-17	0.135	0.138	2.95	0.09	-4.86	-1.65	CAOHIHYLPWYJQM	1049.4	3.5
		november14-18	0.136	0.091	2.99	0.06	-4.91	-1.56	RUQFSDQHKKHMNQ	488.2	2.4
		november14-19	0.140	0.082	3.02	0.05	-4.91	-1.53	GHFRFZROBIWLEQ	641.3	2.8
		november15-20	0.078	0.066	2.83	0.07	-4.84	-1.74	ICKHQKWSFZAMQS	586.2	2.6
		november16-21	0.080	0.075	2.78	0.08	-4.84	-1.84	ICTYZXXAMLSMZ	774.2	2.8

FIGURE 3

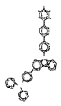
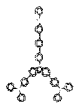
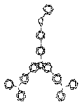
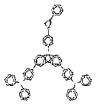
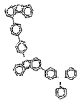
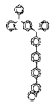
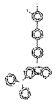
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november17-22	0.161	0.106	2.97	0.03	-4.82	-1.61	HJEZHTUBLLKNRI	728.2	2.7
		november18-23	0.104	0.136	2.81	0.27	-4.78	-1.76	ZSIVNJMPDYMSNL	1021.4	3.1
		november19-24	0.119	0.086	2.81	0.10	-4.75	-1.74	MXCYMNRJWDUVHY	949.4	3.1
		november19-25	0.113	0.061	2.76	0.09	-4.75	-1.76	UWYHBYWETDFUQW	873.3	3.0
		november20-26	0.170	0.102	3.00	0.02	-4.82	-1.59	NIUQWPAPEPLREH	745.3	2.9
		november21-27	0.135	0.089	2.66	0.05	-4.69	-1.84	GSZWWOGYQKJMKW	722.3	2.9
		november22-28	0.075	0.080	2.74	0.47	-4.91	-1.92	IINFHZNIUAQZTC	699.2	2.9

FIGURE 4

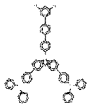
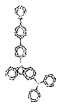
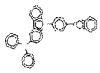
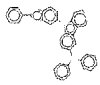
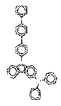
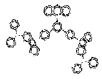
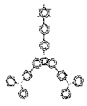
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november23-29	0.112	0.139	2.84	0.21	-4.79	-1.72	BXFCIFOTZUHOKZ	1017.4	3.2
		november24-30	0.109	0.092	2.80	0.13	-4.82	-1.75	VNPSPIXTMNHLTI	565.2	2.6
		november25-31	0.156	0.122	2.75	0.03	-4.90	-1.79	GETCMPAMWKWLEE	528.2	2.5
		november25-32	0.118	0.071	2.76	0.08	-4.84	-1.76	UQWOKUAGDLOXDL	528.2	2.6
		november26-33	0.114	0.087	2.93	0.13	-4.88	-1.65	ADDHRIYICHTVMN	564.2	2.5
		november27-34	0.102	0.124	2.88	0.29	-4.95	-1.77	TYDNWPHNVJZWMA	1089.4	3.7
		november28-35	0.169	0.197	2.93	0.04	-4.78	-1.60	PACRQQOKUSJYJB	971.3	3.1

FIGURE 5

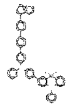
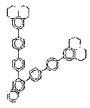
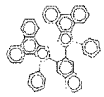
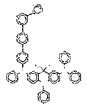
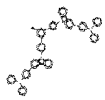
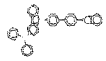
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november29-36	0.150	0.128	2.69	0.04	-4.69	-1.81	DDYZITCVRSXTEI	806.4	3.1
		november30-37	0.133	0.077	2.69	0.05	-4.68	-1.81	MHZQCWSHOKIACJ	808.4	3.1
		november31-38	0.162	0.105	2.66	0.02	-4.73	-1.85	SSPHCUUATALNJT	776.4	2.9
		november32-39	0.137	0.069	2.67	0.04	-5.24	-2.14	DCQWOLCEAXESFD	714.3	2.9
		november33-40	0.168	0.062	2.75	0.01	-4.38	-1.43	JOJBKKZSJKZNOL	854.3	3.2
		november34-41	0.141	0.146	2.91	0.08	-4.85	-1.71	CHPBRFMLSITYII	1071.4	3.4
		november35-42	0.137	0.091	2.67	0.05	-4.87	-1.93	DMKJREFYNMPKLT	620.2	2.7

FIGURE 6

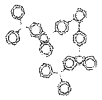
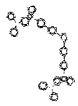
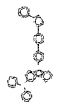
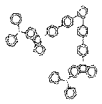
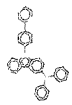
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november36-43	0.162	0.161	2.69	0.03	-5.03	-1.92	IDWOKYWQONPASJ	746.3	3.1
		november36-44	0.094	0.136	2.70	0.38	-4.88	-1.86	XFJYVWAZFXPCMD	898.4	3.3
		november36-45	0.073	0.119	2.72	0.74	-4.88	-1.93	QESUQOXWXXCJAI	1050.4	3.6
		november36-46	0.100	0.083	2.78	0.19	-4.86	-1.81	XDGPYVBACDAWGM	641.3	2.7
		november36-47	0.093	0.081	2.77	0.24	-4.87	-1.86	UMYWCYRSWBKRQB	1050.4	3.6
		november36-48	0.096	0.077	2.70	0.20	-4.89	-1.87	SEGZWZKIVGGCRI	489.2	2.5
		november37-49	0.049	0.086	2.68	1.26	-4.93	-1.98	ZDSVAHGIAOONPY	1036.4	3.5

FIGURE 7

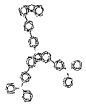
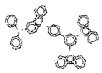
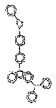
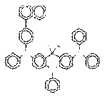
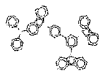
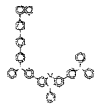
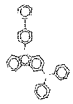
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november38-50	0.162	0.142	2.97	0.03	-4.77	-1.56	UWFPUNSEOLOQFG	988.4	3.4
		november39-51	0.102	0.089	2.92	0.21	-4.88	-1.62	OCKSCLLRPIQMAB	819.3	3.3
		november40-52	0.167	0.147	2.83	0.03	-4.90	-1.79	VQHNEYCDOPWKNC	631.2	2.7
		november41-53	0.164	0.118	2.65	0.02	-4.57	-1.64	VOQQOIVUBVOCTP	747.3	3.1
		november42-54	0.124	0.115	2.90	0.11	-4.96	-1.72	KRKFPQZBVVPGES	819.3	3.2
		november43-55	0.116	0.097	2.66	0.11	-4.61	-1.81	AINPEGXRODPYOW	1051.5	3.5
		november44-56	0.120	0.097	2.76	0.10	-4.93	-1.73	PKBUTJQJPABPCH	489.2	2.5

FIGURE 8

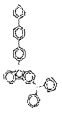
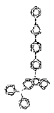
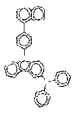
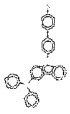
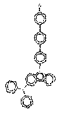
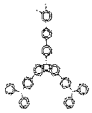
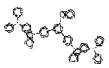
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november44-57	0.106	0.089	2.89	0.18	-4.90	-1.71	CLZZOIONVPYBIP	565.2	2.6
		november44-58	0.099	0.084	2.81	0.21	-4.89	-1.83	TWCHSQCJSKLHHZ	641.3	2.7
		november45-59	0.106	0.068	2.65	0.11	-4.83	-1.89	LXKJQWUOLCXMRB	539.2	2.6
		november46-60	0.136	0.093	3.00	0.06	-4.91	-1.57	BTDMJNDNVMAZEN	555.2	2.5
		november46-61	0.116	0.086	2.95	0.12	-4.88	-1.64	MFFSLRXXODOCIS	631.2	2.6
		november47-62	0.093	0.136	2.74	0.40	-4.81	-1.85	RKYHTSHFVOLHDK	1017.4	3.2
		november48-63	0.123	0.147	2.98	0.16	-4.89	-1.64	CFWTWDZRVXZTBR	1013.4	3.7

FIGURE 9

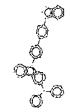
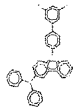
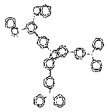
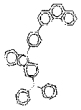
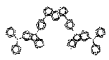
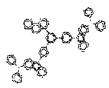
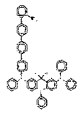
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november48-64	0.124	0.097	2.96	0.10	-4.88	-1.63	XREPFAVDIAQIFV	604.2	2.7
		november49-65	0.087	0.068	2.87	0.28	-4.94	-1.73	YCRPAIZXHXHNGB	623.2	2.8
		november50-66	0.140	0.105	2.93	0.06	-4.80	-1.65	BVTGWVKKOAEQQL	1039.4	3.5
		november51-67	0.143	0.093	2.66	0.04	-4.79	-1.84	ZOWKLDMLDNNSIM	589.2	2.8
		november51-68	0.139	0.066	2.86	0.04	-4.92	-1.78	QDSUYDOFEBBZHR	998.4	3.6
		november51-69	0.152	0.052	2.96	0.02	-4.90	-1.71	BETMSTLDMPLIAA	1074.4	3.9
		november52-70	0.164	0.198	2.67	0.04	-4.40	-1.53	ZGSWOVPBXBKQEA	872.4	3.1

FIGURE 10

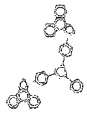
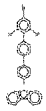
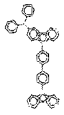
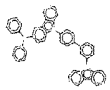
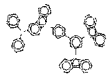
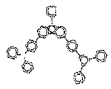
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november53-71	0.077	0.151	2.78	0.85	-5.01	-1.89	KEZXDUHCABQMNN	864.3	3.2
		november54-72	0.152	0.076	2.80	0.02	-5.50	-2.33	MJODJYZDVFEGGF	741.3	2.8
		november55-73	0.169	0.175	2.72	0.03	-5.71	-2.70	LOFFRMGQOCKULH	471.1	2.7
		november56-74	0.145	0.126	2.99	0.06	-4.94	-1.61	DJRSXGCEUWUFMI	554.3	2.8
		november56-75	0.149	0.115	3.02	0.05	-4.94	-1.57	KSJNZFCPVJTGMO	654.3	2.9
		november56-76	0.097	0.102	2.76	0.26	-5.01	-1.92	WTCFYOQFRBVYDK	821.3	3.4
		november57-77	0.148	0.079	2.79	0.03	-4.81	-1.78	KFLYMRHKAJBDBE	793.3	2.7

FIGURE 11

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november57-78	0.141	0.057	2.76	0.03	-4.81	-1.86	QTJYOUSQBXLTOM	869.4	2.6
		november58-79	0.118	0.101	2.69	0.11	-4.84	-1.85	VBFDKGSTTXQPIM	578.2	2.8
		november58-80,malika_June15_12-15	0.121	0.089	2.85	0.10	-4.88	-1.68	OQASBIYZPUPFPV	502.2	2.7
		november58-81	0.165	0.085	2.73	0.02	-4.83	-1.85	ARYSUIAXXDBZBM	654.2	2.9
		november58-82	0.088	0.066	2.85	0.25	-4.85	-1.72	RXLFLXBYZDNCGM	578.2	2.8
		november59-83	0.151	0.161	2.67	0.05	-4.67	-1.81	YYYMCFXXPRKMHA	774.3	2.7
		november60-84	0.133	0.144	3.01	0.11	-4.90	-1.60	YTCCSBXGJKYKOB	1062.3	3.7

FIGURE 12

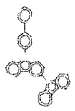
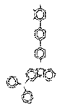
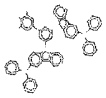
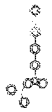
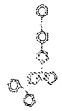
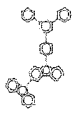
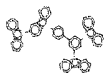
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november61-85	0.161	0.052	3.02	0.01	-5.29	-1.96	QNYROKPJNDTSBD	487.2	2.5
		november62-86	0.163	0.109	3.01	0.03	-4.87	-1.54	XVSULOWNOFQSDR	617.2	2.7
		november62-87	0.053	0.054	2.90	0.80	-5.00	-1.71	AUPBSFCKSJNOQS	874.3	3.3
		november63-88	0.096	0.098	2.81	0.26	-4.88	-1.81	OJLSCPTWQQATHE	703.2	2.7
		november63-89	0.081	0.084	2.79	0.41	-4.91	-1.81	GFOQGOZUKQYYIA	627.2	2.6
		november64-90	0.132	0.059	3.01	0.05	-5.29	-1.99	NIHCWPMKEHXHCQ	639.2	2.7
		november64-91	0.170	0.059	3.23	0.01	-5.34	-1.79	GFMMEODLZMABPM	817.3	3.1

FIGURE 13

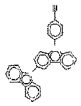
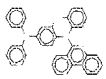
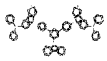
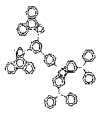
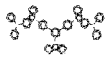
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november65-92	0.138	0.052	3.11	0.04	-5.42	-1.95	YIRWFUCXMDMXPU	434.2	2.4
		november66-93	0.162	0.088	2.66	0.02	-4.77	-1.58	YVBITBFOKHRRAE	543.2	2.6
		november67-94	0.126	0.111	3.00	0.11	-4.91	-1.60	RCKPKGTZDJZPRW	1061.4	3.6
		november68-95	0.118	0.185	2.68	0.20	-4.74	-1.72	PJLQOYKCBXXJET	1085.4	3.6
		november69-96	0.077	0.129	2.65	0.66	-4.67	-1.76	LJQLOVNIZQYYCW	869.3	2.8
		november70-97	0.124	0.152	2.85	0.15	-4.79	-1.63	TZXQPLGCHDOPDS	1061.4	3.6
		november71-98	0.168	0.166	2.98	0.03	-4.83	-1.50	BWGPBUNCCOVNLW	629.2	2.6

FIGURE 14

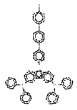
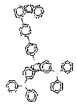
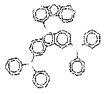
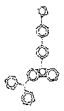
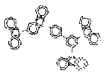
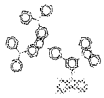
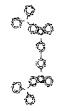
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november72-99	0.132	0.184	2.80	0.13	-4.67	-1.58	XHVZORLQMOWKEN	797.3	2.7
		november73-100	0.105	0.144	2.80	0.28	-4.67	-1.59	HOESFCYVJGPLNW	836.3	3.1
		november73-101	0.077	0.055	2.74	0.30	-4.76	-1.57	PFIUYVCXBUANCU	684.2	2.9
		november74-102	0.142	0.104	2.74	0.05	-4.75	-1.71	KQOBNDLEOXPRBR	553.2	2.6
		november75-103	0.149	0.090	3.05	0.04	-5.29	-1.93	PBVLOOFNAFGVLZ	818.3	3.2
		november76-104	0.149	0.206	2.80	0.07	-4.67	-1.53	VNVNGBSGIPLGKX	985.4	3.5
		november77-105	0.174	0.311	2.65	0.04	-4.79	-1.77	RJFGCAJOVQVUCW	820.3	2.9

FIGURE 15

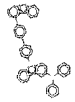
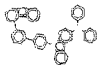
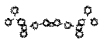
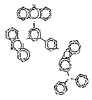
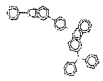
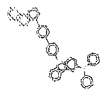
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november78-106	0.103	0.103	2.86	0.22	-4.76	-1.63	PZMZMWBYHNNNJZ	669.2	2.8
		november78-107	0.096	0.081	2.91	0.24	-4.79	-1.57	SHEPWJOCBUHHSC	593.2	2.7
		november78-108	0.121	0.051	3.01	0.06	-4.75	-1.49	MDDJMWOXUJOAPG	669.2	2.8
		november79-109	0.171	0.313	2.79	0.05	-4.72	-1.65	HNUDBAJORCMIFJ	1000.4	3.3
		november80-110	0.113	0.136	2.73	0.19	-4.87	-1.81	UWLMSUAQRBFUQX	872.3	3.0
		november81-111	0.133	0.086	2.66	0.05	-4.71	-1.80	ZRMKIVCVOYROOL	619.2	2.6
		november83-113	0.122	0.095	2.86	0.10	-4.74	-1.63	UJBPURWFLUPDHO	664.3	2.8

FIGURE 16

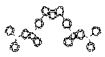
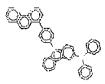
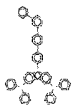
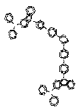
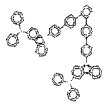
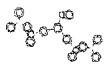
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november83-114	0.115	0.079	2.82	0.11	-4.79	-1.70	VKYASEJWBRPDBU	996.4	3.4
		november83-115	0.129	0.068	2.87	0.05	-4.78	-1.61	IWSQWTDYDNDKNQ	588.2	2.7
		november84-116	0.108	0.112	2.74	0.18	-4.78	-1.74	VYQIYBTZPUGCBC	564.2	2.5
		november85-117	0.166	0.206	2.87	0.04	-4.64	-1.46	ZPHJPBXASRDROU	806.3	2.8
		november86-118	0.082	0.168	2.67	0.71	-4.74	-1.83	RYPFQDBZZHNOOK	1048.4	3.4
		november86-119	0.116	0.120	2.72	0.14	-4.72	-1.74	NTLZOYOZGIWYJY	1048.4	3.4
		november87-120	0.123	0.167	2.92	0.18	-4.73	-1.53	RRXHZLHCLWDQRS	1011.4	3.5

FIGURE 17

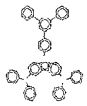
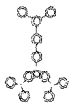
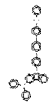
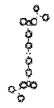
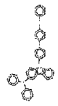
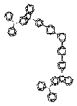
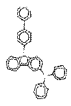
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november86-121	0.134	0.182	2.81	0.12	-4.67	-1.54	PUOATUUYYBDSQC	806.3	2.8
		november88-122	0.146	0.181	2.82	0.07	-4.61	-1.53	UDGRONAKDZFAFQ	882.4	2.9
		november89-123	0.095	0.111	2.74	0.31	-4.75	-1.76	ILDPUAWJUMPPCV	702.2	2.5
		november90-124	0.063	0.156	2.67	1.37	-4.78	-1.85	FRJZLJXAMARHEE	1034.4	3.2
		november90-125	0.107	0.117	2.78	0.20	-4.80	-1.71	QDCVCJOVDBYMSV	626.2	2.4
		november91-126	0.166	0.177	2.88	0.03	-4.70	-1.54	LSXJVTCJNIASRF	1047.4	3.3
		november92-127	0.113	0.099	2.66	0.13	-4.84	-1.84	ZIQLWJIAMVLAIL	468.2	2.4

FIGURE 18

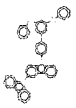
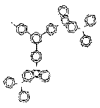
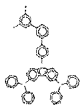
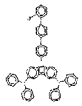
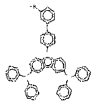
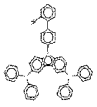
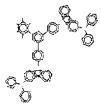
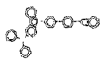
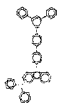
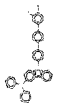
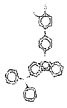
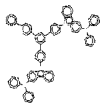
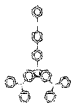
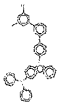
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november93-128	0.150	0.074	3.05	0.03	-5.22	-1.89	AQEQMIBJLIPUGR	764.2	2.7
		november94-129	0.160	0.153	3.00	0.04	-4.76	-1.49	QWVPOUCIWPRPRG	1038.4	3.3
		november95-130	0.099	0.075	2.85	0.19	-4.67	-1.55	BPEYBWPZIFJOOM	865.3	3.0
		november96-131	0.084	0.119	2.69	0.47	-4.62	-1.67	HQFZFXYBOMIRDZ	754.3	2.8
		november96-132	0.113	0.107	2.77	0.15	-4.71	-1.64	IRRMXZDHWCRCO	678.3	2.7
		november96-133	0.090	0.106	2.65	0.33	-4.62	-1.65	QVCCEGKOLSSTKJ	678.3	2.7
		november97-134	0.145	0.126	2.97	0.06	-4.77	-1.52	QGVMPDHPWMTELS	1060.4	3.5

FIGURE 19

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november98-135	0.158	0.162	2.89	0.04	-4.83	-1.59	MEAQBIZQAYRSFD	718.3	3.2
		november99-136	0.142	0.198	2.75	0.09	-4.73	-1.64	JDTDTOUVHBPOAB	985.4	3.5
		november100-137	0.128	0.107	2.68	0.08	-4.69	-1.77	GEGCMGZWSHLJGU	653.2	2.8
		november100-138,malika_June15_10-13	0.112	0.103	2.81	0.15	-4.73	-1.65	QOGBNEZDYUAFTO	577.2	2.7
		november101-139	0.147	0.145	2.88	0.06	-4.84	-1.62	VZOXTPSYRMBAHT	818.3	3.1
		november102-140	0.124	0.079	3.03	0.09	-5.27	-1.95	TYEFFXNXCSPHIB	1026.3	3.3
		november103-141	0.148	0.098	3.03	0.04	-5.30	-1.96	LGASRKWTXZFFNG	770.3	3.0

FIGURE 20

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november104-142	0.121	0.110	2.69	0.11	-4.73	-1.76	URRXEMJFXMAVJV	603.2	2.6
		november105-143	0.115	0.092	2.76	0.12	-4.67	-1.71	ZXTMKRLDMGSHKT	716.3	2.6
		november106-144	0.080	0.097	2.70	0.46	-4.79	-1.83	BVUTWZCFOLLBSG	698.2	2.7
		november106-145	0.091	0.089	2.71	0.27	-4.83	-1.80	RPYCRYYDDQCXQJ	622.2	2.6
		november107-146	0.153	0.057	2.96	0.02	-4.75	-1.55	VOXDXBOLSQFQFJ	1047.4	3.4
		november108-147	0.107	0.161	2.67	0.26	-4.71	-1.73	WFYIXCQYSIAQSD	793.3	2.7
		november109-148	0.119	0.063	2.96	0.08	-4.76	-1.53	UKXMFRAEMKJCAB	698.2	2.7

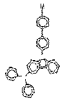
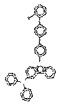
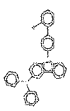
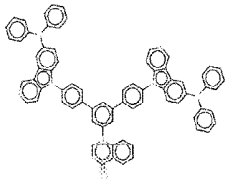
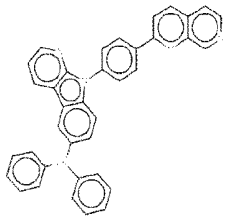
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		november110-149	0.096	0.099	2.66	0.25	-4.82	-1.86	XGWXCZUATCOUES	511.2	2.3
		november110-150	0.084	0.084	2.78	0.36	-4.71	-1.68	QUFCMVFPNRYFNO	587.2	2.5
		november110-151	0.090	0.080	2.78	0.27	-4.75	-1.65	LYHHAJLGSIPVKA	511.2	2.4

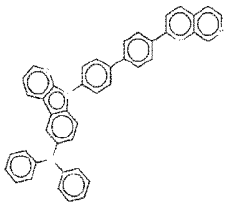
FIGURE 21



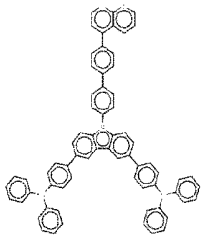
Nickname	november1-1
Splitting	0.097 (eV)
Strength	0.425
Absorption	2.85 (eV)
Rate	0.39 (1/ns)
HOMO	-4.96 (eV)
LUMO	-1.80 (eV)
Key	ZBIAFYAMBDKGJK
Weight	1039.40
SA Score	3.77
Color Est.	



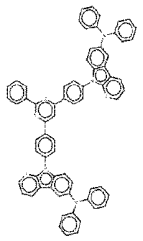
Nickname	november2-2
Splitting	0.150 (eV)
Strength	0.084
Absorption	2.63 (eV)
Rate	0.02 (1/ns)
HOMO	-4.86 (eV)
LUMO	-1.92 (eV)
Key	DVVZYRCIIMRQADO
Weight	539.21
SA Score	2.63
Color Est.	



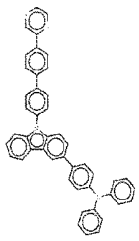
Nickname	november2-3
Splitting	0.153 (eV)
Strength	0.073
Absorption	2.67 (eV)
Rate	0.02 (1/ns)
HOMO	-4.84 (eV)
LUMO	-1.95 (eV)
Key	IYBUKVLNVAWFK
Weight	615.14
SA Score	2.76
Color Est.	



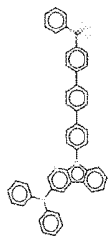
Nickname	november3-4
Splitting	0.040 (eV)
Strength	0.057
Absorption	2.69 (eV)
Rate	1.16 (1/ns)
HOMO	-4.80 (eV)
LUMO	-1.91 (eV)
Key	ANF5AKQBNKHQU
Weight	933.38
SA Score	3.17
Color Est.	



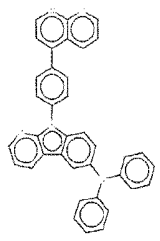
Nickname	november4-5
Splitting	0.129 (eV)
Strength	0.288
Absorption	2.82 (eV)
Rate	0.22 (1/ns)
HOMO	-4.87 (eV)
LUMO	-1.74 (eV)
Key	BBYZHFAMUHQQH
Weight	974.38
SA Score	3.43
Color Est.	



Nickname	november5-6
Splitting	0.114 (eV)
Strength	0.080
Absorption	2.80 (eV)
Rate	0.11 (1/ns)
HOMO	-4.80 (eV)
LUMO	-1.79 (eV)
Key	RJUKARAKVZRMG
Weight	640.26
SA Score	2.64
Color Est.	



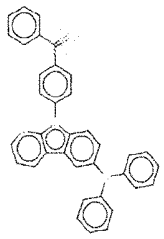
Nickname	november6-7
Splitting	0.160 (eV)
Strength	0.084
Absorption	2.86 (eV)
Rate	0.02 (1/ns)
HOMO	-4.91 (eV)
LUMO	-1.85 (eV)
Key	UZFQNZNBHGSH
Weight	667.26
SA Score	2.65
Color Est.	



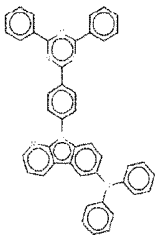
Nickname	november7-8
Splitting	0.113 (eV)
Strength	0.065
Absorption	2.85 (eV)
Rate	0.10 (1/ns)
HOMO	-4.94 (eV)
LUMO	-1.80 (eV)
Key	HOIYRWPDLXVUOQ
Weight	539.21
SA Score	2.64
Color Est.	

Table 2

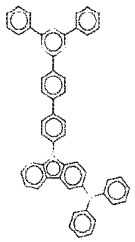
FIGURE 22



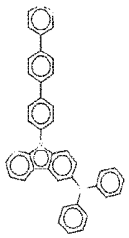
Nickname	november8-9
Splitting	0.166 (eV)
Strength	0.114
Absorption	2.83 (eV)
Rate	0.02 (1/ns)
HOMO	-4.90 (eV)
LUMO	-1.73 (eV)
Key	XPRNLFUWIXGSI
Weight	515.20
SA Score	2.37
Color Est.	



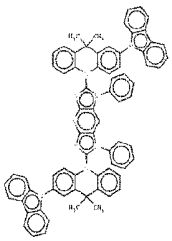
Nickname	november9-10
Splitting	0.138 (eV)
Strength	0.165
Absorption	2.72 (eV)
Rate	0.09 (1/ns)
HOMO	-4.87 (eV)
LUMO	-1.84 (eV)
Key	JBSCTKNWQJVOFC
Weight	642.25
SA Score	2.67
Color Est.	



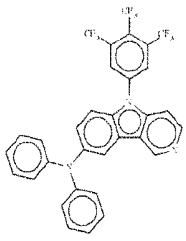
Nickname	november9-11
Splitting	0.087 (eV)
Strength	0.164
Absorption	2.76 (eV)
Rate	0.38 (1/ns)
HOMO	-4.84 (eV)
LUMO	-1.90 (eV)
Key	GMDPSGRZVQDVGJ
Weight	718.28
SA Score	2.77
Color Est.	



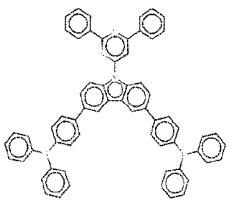
Nickname	november10-12
Splitting	0.159 (eV)
Strength	0.109
Absorption	2.85 (eV)
Rate	0.03 (1/ns)
HOMO	-4.91 (eV)
LUMO	-1.81 (eV)
Key	CBVBCCPDBALXHL
Weight	865.23
SA Score	2.67
Color Est.	



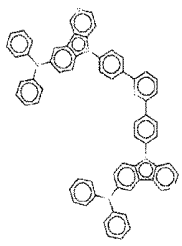
Nickname	november11-13
Splitting	0.174 (eV)
Strength	0.121
Absorption	3.17 (eV)
Rate	0.02 (1/ns)
HOMO	-5.14 (eV)
LUMO	-1.49 (eV)
Key	PBOQMQHRHKGLNX
Weight	1055.44
SA Score	3.90
Color Est.	



Nickname	november12-14
Splitting	0.150 (eV)
Strength	0.089
Absorption	2.69 (eV)
Rate	0.03 (1/ns)
HOMO	-5.14 (eV)
LUMO	-2.07 (eV)
Key	IGEGOLRVNRZJDF
Weight	615.14
SA Score	2.96
Color Est.	

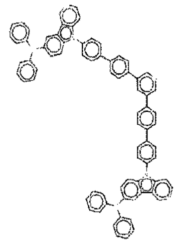


Nickname	november13-15
Splitting	0.117 (eV)
Strength	0.060
Absorption	2.85 (eV)
Rate	0.08 (1/ns)
HOMO	-4.81 (eV)
LUMO	-1.56 (eV)
Key	JKHHZAYXVCJFJ
Weight	883.37
SA Score	2.97
Color Est.	

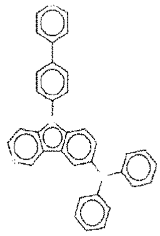


Nickname	november14-16
Splitting	0.147 (eV)
Strength	0.157
Absorption	2.90 (eV)
Rate	0.06 (1/ns)
HOMO	-4.87 (eV)
LUMO	-1.64 (eV)
Key	VMWHUNGZOUTRRI
Weight	897.36
SA Score	4.25
Color Est.	

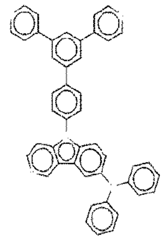
FIGURE 23



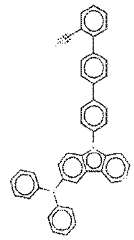
Nickname	november14-17
Splitting	0.135 (eV)
Strength	0.138
Absorption	2.95 (eV)
Rate	0.09 (1 us)
HOMO	-4.88 (eV)
LUMO	-1.65 (eV)
Key	CAOIEHYL4PWYJQM
Weight	1049.42
SA Score	3.50
Color Est.:	



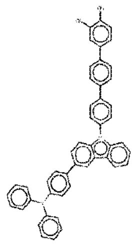
Nickname	november14-18
Splitting	0.136 (eV)
Strength	0.091
Absorption	2.99 (eV)
Rate	0.06 (1 us)
HOMO	-4.91 (eV)
LUMO	-1.56 (eV)
Key	RUQFSDQHKKHMNQ
Weight	488.20
SA Score	2.43
Color Est.:	



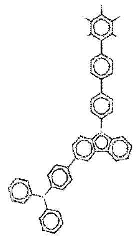
Nickname	november14-19
Splitting	0.140 (eV)
Strength	0.082
Absorption	3.02 (eV)
Rate	0.05 (1 us)
HOMO	-4.91 (eV)
LUMO	-1.63 (eV)
Key	GHFRFZPOBIWLEQ
Weight	641.26
SA Score	2.77
Color Est.:	



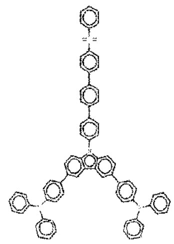
Nickname	november15-20
Splitting	0.078 (eV)
Strength	0.066
Absorption	2.83 (eV)
Rate	0.37 (1 us)
HOMO	-4.84 (eV)
LUMO	-1.74 (eV)
Key	ICKHQKWSFZAMQS
Weight	588.23
SA Score	2.64
Color Est.:	



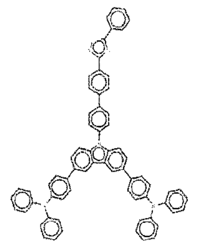
Nickname	november16-21
Splitting	0.080 (eV)
Strength	0.075
Absorption	2.78 (eV)
Rate	0.38 (1 us)
HOMO	-4.84 (eV)
LUMO	-1.84 (eV)
Key	ICTYZXXXAMLSMZ
Weight	774.25
SA Score	2.78
Color Est.:	



Nickname	november17-22
Splitting	0.161 (eV)
Strength	0.106
Absorption	2.97 (eV)
Rate	0.03 (1 us)
HOMO	-4.82 (eV)
LUMO	-1.61 (eV)
Key	HIEZHTUBLLKNRI
Weight	728.23
SA Score	2.72
Color Est.:	

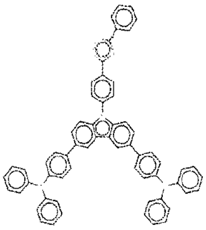


Nickname	november18-23
Splitting	0.104 (eV)
Strength	0.136
Absorption	2.81 (eV)
Rate	0.27 (1 us)
HOMO	-4.78 (eV)
LUMO	-1.76 (eV)
Key	ZSIVNJMPDYMSNL
Weight	1021.37
SA Score	3.11
Color Est.:	

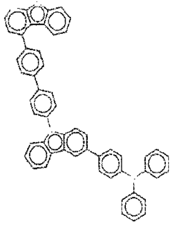


Nickname	november19-24
Splitting	0.119 (eV)
Strength	0.086
Absorption	2.81 (eV)
Rate	0.10 (1 us)
HOMO	-4.75 (eV)
LUMO	-1.74 (eV)
Key	MXCYMNRJWDUVHY
Weight	949.38
SA Score	3.14
Color Est.:	

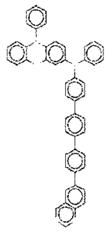
FIGURE 24



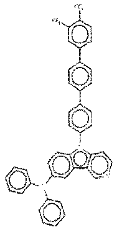
Nickname	november19-25
Splitting	0.113 (eV)
Strength	0.061
Absorption	2.76 (eV)
Rate	0.09 (1 us)
HOMO	-4.75 (eV)
LUMO	-1.76 (eV)
Key	UWYHBYWHTDFUQW
Weight	873.35
SA Score	3.06
Color Est.	



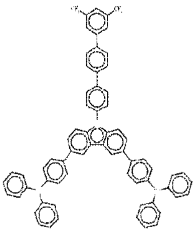
Nickname	november20-26
Splitting	0.170 (eV)
Strength	0.102
Absorption	3.00 (eV)
Rate	0.02 (1 us)
HOMO	-4.82 (eV)
LUMO	-1.59 (eV)
Key	NILQWPAPFPLRFFI
Weight	746.26
SA Score	2.92
Color Est.	



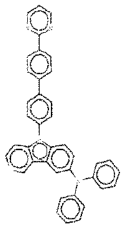
Nickname	november21-27
Splitting	0.135 (eV)
Strength	0.089
Absorption	2.66 (eV)
Rate	0.05 (1 us)
HOMO	-4.69 (eV)
LUMO	-1.84 (eV)
Key	GSZWWOGYQKJMKW
Weight	722.25
SA Score	2.92
Color Est.	



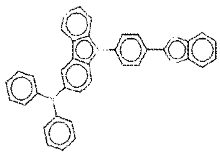
Nickname	november22-28
Splitting	0.075 (eV)
Strength	0.080
Absorption	2.74 (eV)
Rate	0.47 (1 us)
HOMO	-4.91 (eV)
LUMO	-1.92 (eV)
Key	BNFHZNIUAQZTQ
Weight	699.21
SA Score	2.91
Color Est.	



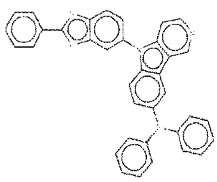
Nickname	november23-29
Splitting	0.112 (eV)
Strength	0.139
Absorption	2.84 (eV)
Rate	0.21 (1 us)
HOMO	-4.79 (eV)
LUMO	-1.72 (eV)
Key	BXFCHOTZUHOKZ
Weight	1017.35
SA Score	3.20
Color Est.	



Nickname	november24-30
Splitting	0.109 (eV)
Strength	0.082
Absorption	2.80 (eV)
Rate	0.13 (1 us)
HOMO	-4.82 (eV)
LUMO	-1.75 (eV)
Key	VNPSPIXTMNHLTI
Weight	565.23
SA Score	2.51
Color Est.	

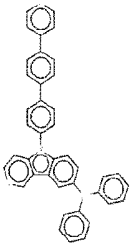


Nickname	november25-31
Splitting	0.156 (eV)
Strength	0.122
Absorption	2.75 (eV)
Rate	0.03 (1 us)
HOMO	-4.90 (eV)
LUMO	-1.79 (eV)
Key	GHTCMPAMWKWLEE
Weight	528.20
SA Score	2.54
Color Est.	

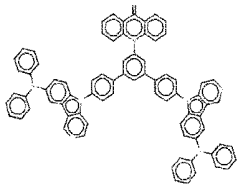


Nickname	november25-32
Splitting	0.118 (eV)
Strength	0.071
Absorption	2.76 (eV)
Rate	0.08 (1 us)
HOMO	-4.84 (eV)
LUMO	-1.76 (eV)
Key	UQWQKUAGDLDXDL
Weight	528.20
SA Score	2.58
Color Est.	

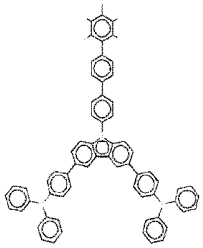
FIGURE 25



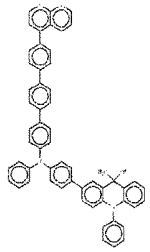
Nickname	november26-33
Splitting	0.114 (eV)
Strength	0.087
Absorption	2.93 (eV)
Rate	0.13 (1/ns)
HOMO	-4.88 (eV)
LUMO	-1.65 (eV)
Key	ADCHRIYICHTVMN
Weight	564.23
SA Score	2.51
Color Est.:	



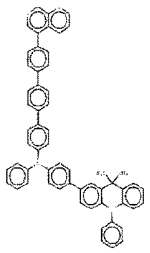
Nickname	november27-34
Splitting	0.102 (eV)
Strength	0.124
Absorption	2.88 (eV)
Rate	0.29 (1/ns)
HOMO	-4.95 (eV)
LUMO	-1.77 (eV)
Key	TYBNWPHNVZWMA
Weight	1089.42
SA Score	3.74
Color Est.:	



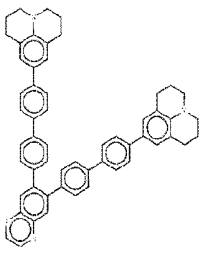
Nickname	november28-35
Splitting	0.169 (eV)
Strength	0.197
Absorption	2.93 (eV)
Rate	0.04 (1/ns)
HOMO	-4.78 (eV)
LUMO	-1.60 (eV)
Key	PACRQQCKUSIYJB
Weight	971.33
SA Score	3.13
Color Est.:	



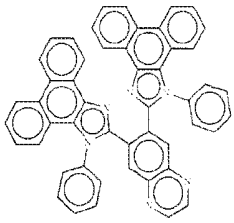
Nickname	november29-36
Splitting	0.150 (eV)
Strength	0.128
Absorption	2.69 (eV)
Rate	0.04 (1/ns)
HOMO	-4.69 (eV)
LUMO	-1.81 (eV)
Key	DDYZTTCVRSNTEJ
Weight	808.36
SA Score	3.09
Color Est.:	



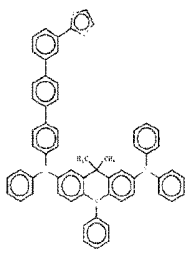
Nickname	november30-37
Splitting	0.133 (eV)
Strength	0.077
Absorption	2.69 (eV)
Rate	0.05 (1/ns)
HOMO	-4.68 (eV)
LUMO	-1.81 (eV)
Key	XJTZQUWSHOKIAGJ
Weight	808.36
SA Score	3.13
Color Est.:	



Nickname	november31-38
Splitting	0.162 (eV)
Strength	0.105
Absorption	2.66 (eV)
Rate	0.02 (1/ns)
HOMO	-4.73 (eV)
LUMO	-1.85 (eV)
Key	SSPTICUUATALNJT
Weight	776.39
SA Score	2.90
Color Est.:	

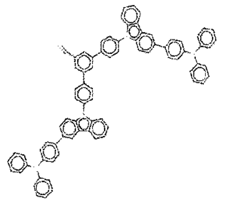


Nickname	november32-39
Splitting	0.137 (eV)
Strength	0.069
Absorption	2.67 (eV)
Rate	0.04 (1/ns)
HOMO	-5.24 (eV)
LUMO	-2.14 (eV)
Key	IWQWDLCEAXESED
Weight	714.25
SA Score	2.88
Color Est.:	

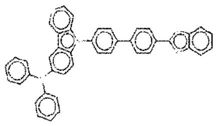


Nickname	november33-40
Splitting	0.168 (eV)
Strength	0.062
Absorption	2.75 (eV)
Rate	0.01 (1/ns)
HOMO	-4.38 (eV)
LUMO	-1.43 (eV)
Key	BOBKKZSHKZSNOL
Weight	854.34
SA Score	3.18
Color Est.:	

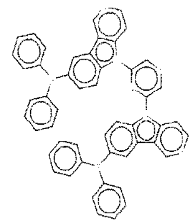
FIGURE 26



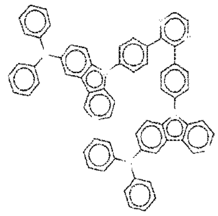
Nickname	november34-41
Splitting	0.141 (eV)
Strength	0.146
Absorption	2.91 (eV)
Rate	0.08 (1 us)
HOMO	-4.85 (eV)
LUMO	-1.71 (eV)
Key	CHPBRFMLSITYH
Weight	1071.43
SA Score	3.44
Color Est..	



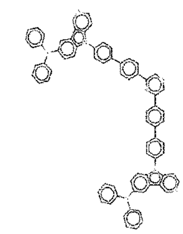
Nickname	november35-42
Splitting	0.137 (eV)
Strength	0.091
Absorption	2.67 (eV)
Rate	0.05 (1 us)
HOMO	-4.87 (eV)
LUMO	-1.93 (eV)
Key	DMKJRFFYNMPKLT
Weight	620.20
SA Score	2.67
Color Est..	



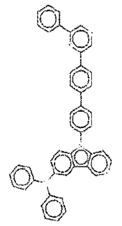
Nickname	november36-43
Splitting	0.162 (eV)
Strength	0.161
Absorption	2.69 (eV)
Rate	0.03 (1 us)
HOMO	-5.03 (eV)
LUMO	-1.92 (eV)
Key	IDWQKYWQONFASJ
Weight	746.29
SA Score	3.18
Color Est..	



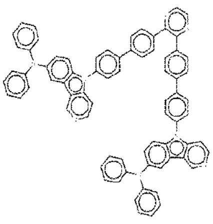
Nickname	november16-44
Splitting	0.094 (eV)
Strength	0.136
Absorption	2.70 (eV)
Rate	0.38 (1 us)
HOMO	-4.88 (eV)
LUMO	-1.86 (eV)
Key	NFJYVWAZFXPCMD
Weight	898.35
SA Score	3.29
Color Est..	



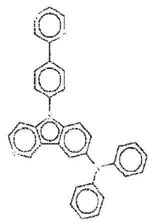
Nickname	november36-45
Splitting	0.073 (eV)
Strength	0.119
Absorption	2.72 (eV)
Rate	0.74 (1 us)
HOMO	-4.88 (eV)
LUMO	-1.93 (eV)
Key	QESUQOXWXXCIAI
Weight	1050.42
SA Score	3.57
Color Est..	



Nickname	november36-46
Splitting	0.100 (eV)
Strength	0.083
Absorption	2.78 (eV)
Rate	0.19 (1 us)
HOMO	-4.86 (eV)
LUMO	-1.81 (eV)
Key	NDGPVVBACDAWGM
Weight	641.26
SA Score	2.73
Color Est..	

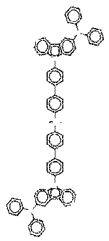


Nickname	november36-47
Splitting	0.093 (eV)
Strength	0.081
Absorption	2.77 (eV)
Rate	0.24 (1 us)
HOMO	-4.87 (eV)
LUMO	-1.86 (eV)
Key	CMYWCYRSWBKRQB
Weight	1050.42
SA Score	3.56
Color Est..	

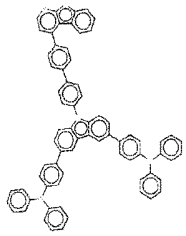


Nickname	november36-48
Splitting	0.096 (eV)
Strength	0.077
Absorption	2.70 (eV)
Rate	0.20 (1 us)
HOMO	-4.89 (eV)
LUMO	-1.87 (eV)
Key	SEGZWZKIVGGCRI
Weight	489.20
SA Score	2.52
Color Est..	

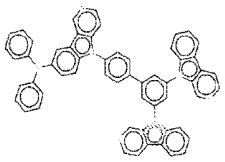
FIGURE 27



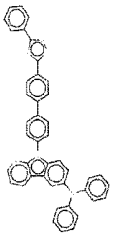
Nickname	november37-49
Splitting	0.049 (eV)
Strength	0.086
Absorption	2.68 (eV)
Rate	1.26 (1/ns)
HOMO	-4.93 (eV)
LUMO	-1.98 (eV)
Key	ZDSVAIRGLAOQNPV
Weight	1036.36
SA Score	3.47
Color Est.:	



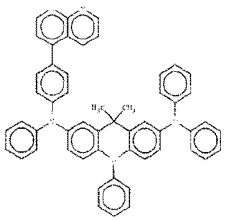
Nickname	november38-50
Splitting	0.162 (eV)
Strength	0.142
Absorption	2.97 (eV)
Rate	0.03 (1/ns)
HOMO	-4.77 (eV)
LUMO	-1.56 (eV)
Key	CVFDLNSRCLOQAG
Weight	988.36
SA Score	3.37
Color Est.:	



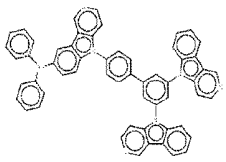
Nickname	november39-51
Splitting	0.102 (eV)
Strength	0.089
Absorption	2.92 (eV)
Rate	0.21 (1/ns)
HOMO	-4.88 (eV)
LUMO	-1.62 (eV)
Key	OCKSCLLRPQMAB
Weight	819.31
SA Score	3.27
Color Est.:	



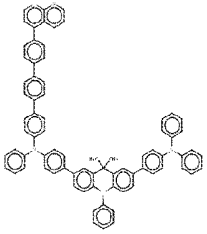
Nickname	november40-52
Splitting	0.167 (eV)
Strength	0.147
Absorption	2.83 (eV)
Rate	0.03 (1/ns)
HOMO	-4.90 (eV)
LUMO	-1.79 (eV)
Key	VQHNEVGDOPWENO
Weight	631.24
SA Score	2.70
Color Est.:	



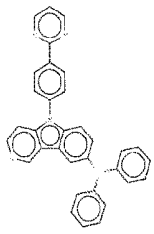
Nickname	november41-53
Splitting	0.164 (eV)
Strength	0.118
Absorption	2.65 (eV)
Rate	0.02 (1/ns)
HOMO	-4.87 (eV)
LUMO	-1.64 (eV)
Key	VDQQOVUBVOCTP
Weight	747.34
SA Score	3.05
Color Est.:	



Nickname	november42-54
Splitting	0.124 (eV)
Strength	0.115
Absorption	2.80 (eV)
Rate	0.11 (1/ns)
HOMO	-4.96 (eV)
LUMO	-1.72 (eV)
Key	KRKFPGZBVVPGES
Weight	819.31
SA Score	3.23
Color Est.:	

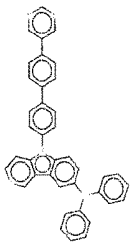


Nickname	november43-55
Splitting	0.116 (eV)
Strength	0.097
Absorption	2.66 (eV)
Rate	0.11 (1/ns)
HOMO	-4.61 (eV)
LUMO	-1.81 (eV)
Key	AINPBGXROUPYQW
Weight	1051.46
SA Score	3.55
Color Est.:	

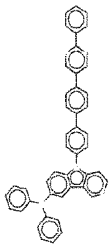


Nickname	november44-56
Splitting	0.120 (eV)
Strength	0.097
Absorption	2.76 (eV)
Rate	0.10 (1/ns)
HOMO	-4.83 (eV)
LUMO	-1.73 (eV)
Key	PKBUTLQBABPCH
Weight	489.20
SA Score	2.49
Color Est.:	

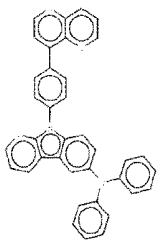
FIGURE 28



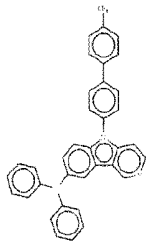
Nickname	november44-57
Splitting	0.106 (eV)
Strength	0.089
Absorption	2.89 (eV)
Rate	0.18 (1/fs)
HOMO	-4.90 (eV)
LUMO	-1.71 (eV)
Key	CLZZFRONVPVHP
Weight	563.23
SA Score	2.64
Color Est.	



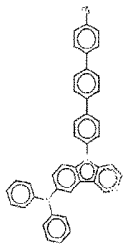
Nickname	november44-58
Splitting	0.099 (eV)
Strength	0.084
Absorption	2.81 (eV)
Rate	0.21 (1/fs)
HOMO	-4.89 (eV)
LUMO	-1.83 (eV)
Key	TWCHSQOSKLHHZ
Weight	641.26
SA Score	2.71
Color Est.	



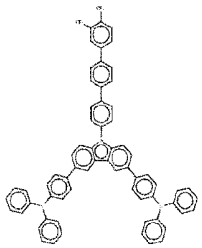
Nickname	november45-59
Splitting	0.106 (eV)
Strength	0.068
Absorption	2.65 (eV)
Rate	0.11 (1/fs)
HOMO	-4.83 (eV)
LUMO	-1.89 (eV)
Key	LNKJQWUOLCNMRB
Weight	539.21
SA Score	2.62
Color Est.	



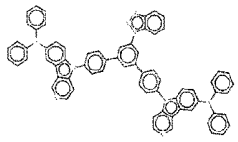
Nickname	november46-60
Splitting	0.136 (eV)
Strength	0.093
Absorption	3.00 (eV)
Rate	0.06 (1/fs)
HOMO	-4.91 (eV)
LUMO	-1.57 (eV)
Key	BTDMJNDNVMAZEN
Weight	555.19
SA Score	2.52
Color Est.	



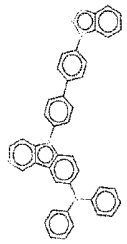
Nickname	november46-61
Splitting	0.116 (eV)
Strength	0.086
Absorption	2.95 (eV)
Rate	0.12 (1/fs)
HOMO	-4.88 (eV)
LUMO	-1.64 (eV)
Key	MFFSLRXXOHCYIS
Weight	634.22
SA Score	2.65
Color Est.	



Nickname	november47-62
Splitting	0.093 (eV)
Strength	0.136
Absorption	2.74 (eV)
Rate	0.40 (1/fs)
HOMO	-4.81 (eV)
LUMO	-1.85 (eV)
Key	RKYITSIBVOLHDK
Weight	1017.35
SA Score	3.22
Color Est.	

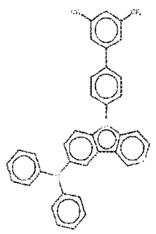


Nickname	november48-63
Splitting	0.123 (eV)
Strength	0.147
Absorption	2.99 (eV)
Rate	0.16 (1/fs)
HOMO	-4.89 (eV)
LUMO	-1.64 (eV)
Key	CPWTWDZRVXZTBR
Weight	1013.40
SA Score	3.67
Color Est.	

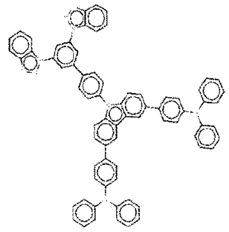


Nickname	november48-64
Splitting	0.124 (eV)
Strength	0.097
Absorption	2.96 (eV)
Rate	0.10 (1/fs)
HOMO	-4.88 (eV)
LUMO	-1.63 (eV)
Key	XREHFAVDIAQTFV
Weight	604.24
SA Score	2.72
Color Est.	

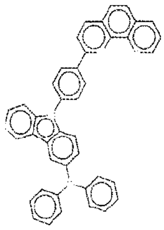
FIGURE 29



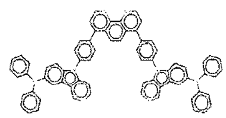
Nickname	november49-65
Splitting	0.087 (eV)
Strength	0.068
Absorption	2.87 (eV)
Rate	0.28 (1 us)
HOMO	-4.94 (eV)
LUMO	-1.73 (eV)
Key	YCRPAIZXHXHNGB
Weight	623.18
SA Score	2.77
Color Est.:	



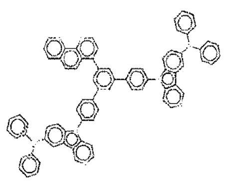
Nickname	november50-66
Splitting	0.140 (eV)
Strength	0.165
Absorption	2.93 (eV)
Rate	0.06 (1 us)
HOMO	-4.80 (eV)
LUMO	-1.65 (eV)
Key	BVTOWVKKOAEQQL
Weight	1039.41
SA Score	3.52
Color Est.:	



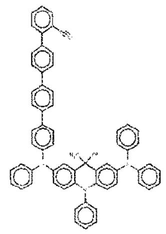
Nickname	november51-67
Splitting	0.143 (eV)
Strength	0.693
Absorption	2.66 (eV)
Rate	0.04 (1 us)
HOMO	-4.79 (eV)
LUMO	-1.84 (eV)
Key	ZOWKLDMLDNNSIM
Weight	589.23
SA Score	2.75
Color Est.:	



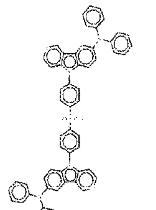
Nickname	november51-68
Splitting	0.139 (eV)
Strength	0.066
Absorption	2.86 (eV)
Rate	0.04 (1 us)
HOMO	-4.92 (eV)
LUMO	-1.78 (eV)
Key	QDSUYDOPFBBZHR
Weight	998.38
SA Score	3.60
Color Est.:	



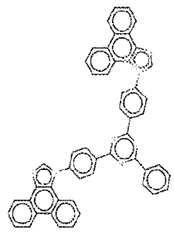
Nickname	november51-69
Splitting	0.152 (eV)
Strength	0.052
Absorption	2.96 (eV)
Rate	0.02 (1 us)
HOMO	-4.98 (eV)
LUMO	-1.71 (eV)
Key	BETMSTLDMPLIAA
Weight	1074.42
SA Score	3.89
Color Est.:	



Nickname	november52-70
Splitting	0.164 (eV)
Strength	0.198
Absorption	2.67 (eV)
Rate	0.04 (1 us)
HOMO	-4.40 (eV)
LUMO	-1.53 (eV)
Key	ZGSWQVPBNBKQEA
Weight	872.39
SA Score	3.11
Color Est.:	

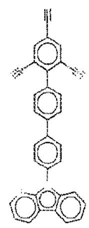


Nickname	november53-71
Splitting	0.077 (eV)
Strength	0.151
Absorption	2.78 (eV)
Rate	0.85 (1 us)
HOMO	-5.01 (eV)
LUMO	-1.69 (eV)
Key	KEZNDUHCABQMNN
Weight	884.29
SA Score	3.17
Color Est.:	

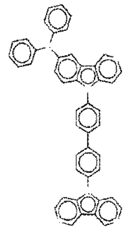


Nickname	november54-72
Splitting	0.132 (eV)
Strength	0.076
Absorption	2.80 (eV)
Rate	0.02 (1 us)
HOMO	-5.50 (eV)
LUMO	-2.33 (eV)
Key	MIODIYZDVFEGGF
Weight	741.26
SA Score	2.78
Color Est.:	

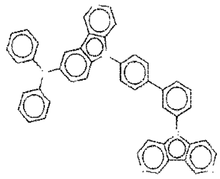
FIGURE 30



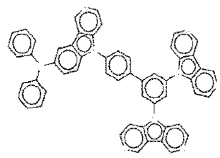
Nickname	november55-73
Splitting	0.169 (eV)
Strength	0.175
Absorption	2.72 (eV)
Rate	0.03 (1 us)
HOMO	-5.71 (eV)
LUMO	-2.70 (eV)
Key	LOHHXMGQOCKULH
Weight	471.15
SA Score	2.66
Color Est.	



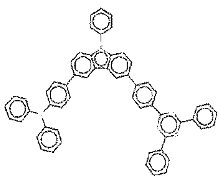
Nickname	november56-74
Splitting	0.145 (eV)
Strength	0.126
Absorption	2.99 (eV)
Rate	0.06 (1 us)
HOMO	-4.94 (eV)
LUMO	-1.61 (eV)
Key	DJRSNGCRWUFMI
Weight	654.25
SA Score	2.78
Color Est.	



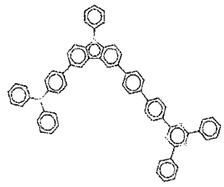
Nickname	november56-75
Splitting	0.149 (eV)
Strength	0.115
Absorption	3.02 (eV)
Rate	0.05 (1 us)
HOMO	-4.94 (eV)
LUMO	-1.57 (eV)
Key	KSJNZFCPVJTGMO
Weight	654.25
SA Score	2.91
Color Est.	



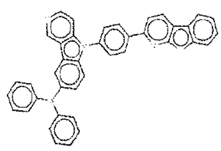
Nickname	november56-76
Splitting	0.097 (eV)
Strength	0.102
Absorption	2.76 (eV)
Rate	0.26 (1 us)
HOMO	-5.01 (eV)
LUMO	-1.92 (eV)
Key	WTCFYOQFRBVYDK
Weight	821.30
SA Score	3.35
Color Est.	



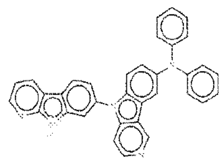
Nickname	november57-77
Splitting	0.148 (eV)
Strength	0.079
Absorption	2.79 (eV)
Rate	0.03 (1 us)
HOMO	-4.81 (eV)
LUMO	-1.78 (eV)
Key	KFLYMRFKAJBDBE
Weight	793.32
SA Score	2.67
Color Est.	



Nickname	november57-78
Splitting	0.141 (eV)
Strength	0.057
Absorption	2.76 (eV)
Rate	0.03 (1 us)
HOMO	-4.81 (eV)
LUMO	-1.86 (eV)
Key	QTJYOUSQBXLTOM
Weight	869.35
SA Score	2.80
Color Est.	

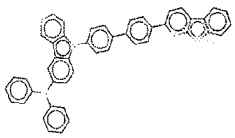


Nickname	november58-79
Splitting	0.118 (eV)
Strength	0.101
Absorption	2.68 (eV)
Rate	0.11 (1 us)
HOMO	-4.84 (eV)
LUMO	-1.85 (eV)
Key	YBFDKGSTTNQPIM
Weight	578.21
SA Score	2.76
Color Est.	

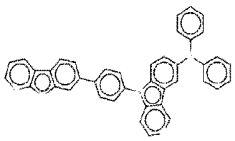


Nickname	november58_june15_12-15
Splitting	0.121 (eV)
Strength	0.089
Absorption	2.85 (eV)
Rate	0.10 (1 us)
HOMO	-4.88 (eV)
LUMO	-1.68 (eV)
Key	OQASBIYZPUTFPV
Weight	502.18
SA Score	2.70
Color Est.	

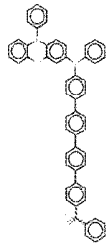
FIGURE 31



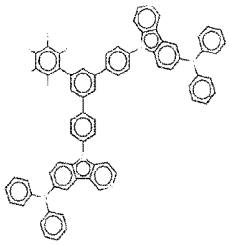
Nickname	november58-81
Splitting	0.165 (eV)
Strength	0.083
Absorption	2.73 (eV)
Rate	0.02 (1/ns)
HOMO	-4.83 (eV)
LUMO	-1.85 (eV)
Key	ARYSUTAXXDRZBM
Weight	654.24
SA Score	2.89
Color Est.:	



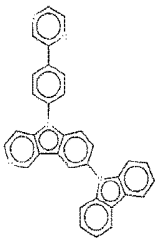
Nickname	november58-82
Splitting	0.088 (eV)
Strength	0.066
Absorption	2.85 (eV)
Rate	0.25 (1/ns)
HOMO	-4.85 (eV)
LUMO	-1.72 (eV)
Key	RXLHXBVZDNCGM
Weight	578.21
SA Score	2.80
Color Est.:	



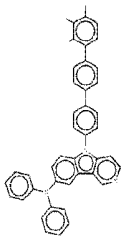
Nickname	november59-83
Splitting	0.151 (eV)
Strength	0.161
Absorption	2.67 (eV)
Rate	0.95 (1/ns)
HOMO	-4.67 (eV)
LUMO	-1.81 (eV)
Key	YVYMCFNXPRKMHA
Weight	774.27
SA Score	2.74
Color Est.:	



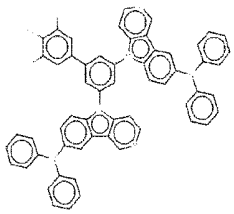
Nickname	november60-84
Splitting	0.133 (eV)
Strength	0.144
Absorption	3.01 (eV)
Rate	0.11 (1/ns)
HOMO	-4.90 (eV)
LUMO	-1.68 (eV)
Key	YTCCSBXGJKYEOB
Weight	1062.35
SA Score	3.72
Color Est.:	



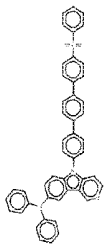
Nickname	november61-85
Splitting	0.161 (eV)
Strength	0.052
Absorption	3.02 (eV)
Rate	0.01 (1/ns)
HOMO	-5.29 (eV)
LUMO	-1.96 (eV)
Key	QNYROKPJNDTSBD
Weight	407.18
SA Score	2.52
Color Est.:	



Nickname	november62-86
Splitting	0.163 (eV)
Strength	0.109
Absorption	3.01 (eV)
Rate	0.03 (1/ns)
HOMO	-4.87 (eV)
LUMO	-1.54 (eV)
Key	YVSUFOWNOPQNDR
Weight	617.21
SA Score	2.71
Color Est.:	

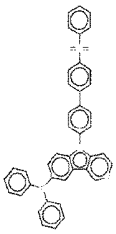


Nickname	november62-87
Splitting	0.053 (eV)
Strength	0.054
Absorption	2.90 (eV)
Rate	0.80 (1/ns)
HOMO	-5.09 (eV)
LUMO	-1.71 (eV)
Key	AUPRSFCKSJNOQS
Weight	874.30
SA Score	3.34
Color Est.:	

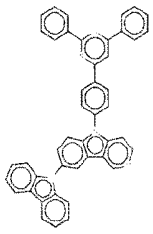


Nickname	november63-88
Splitting	0.096 (eV)
Strength	0.098
Absorption	2.81 (eV)
Rate	0.28 (1/ns)
HOMO	-4.88 (eV)
LUMO	-1.80 (eV)
Key	OILBCPTWQQATHE
Weight	703.23
SA Score	2.72
Color Est.:	

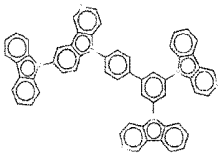
FIGURE 32



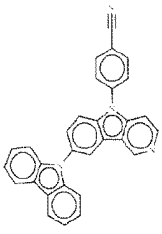
Nickname	november63-89
Splitting	0.081 (eV)
Strength	0.084
Absorption	2.79 (eV)
Rate	0.41 (1/ns)
HOMO	-4.91 (eV)
LUMO	-1.81 (eV)
Key	GEOQGOZFKQYYIA
Weight	627.20
SA Score	2.63
Color Est.	



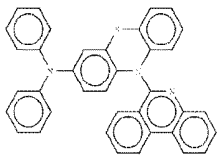
Nickname	november64-90
Splitting	0.132 (eV)
Strength	0.059
Absorption	3.01 (eV)
Rate	0.05 (1/ns)
HOMO	-5.29 (eV)
LUMO	-1.99 (eV)
Key	NHCWPMKEHXHCQ
Weight	639.24
SA Score	2.65
Color Est.	



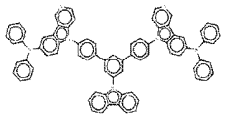
Nickname	november64-91
Splitting	0.170 (eV)
Strength	0.059
Absorption	3.23 (eV)
Rate	0.01 (1/ns)
HOMO	-5.34 (eV)
LUMO	-1.79 (eV)
Key	OFNMBODFZMABFM
Weight	817.30
SA Score	3.10
Color Est.	



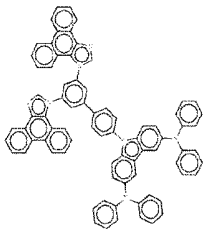
Nickname	november65-92
Splitting	0.138 (eV)
Strength	0.052
Absorption	3.11 (eV)
Rate	0.04 (1/ns)
HOMO	-5.42 (eV)
LUMO	-1.95 (eV)
Key	YBWFFCXGBMXPC
Weight	484.15
SA Score	2.37
Color Est.	



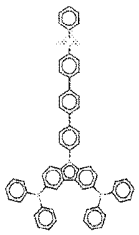
Nickname	november66-93
Splitting	0.162 (eV)
Strength	0.088
Absorption	2.66 (eV)
Rate	0.02 (1/ns)
HOMO	-4.77 (eV)
LUMO	-1.58 (eV)
Key	YWBTBROKHRRAE
Weight	543.18
SA Score	2.61
Color Est.	



Nickname	november67-94
Splitting	0.126 (eV)
Strength	0.114
Absorption	3.00 (eV)
Rate	0.11 (1/ns)
HOMO	-4.91 (eV)
LUMO	-1.60 (eV)
Key	RCKPKGTZDTZHRW
Weight	1061.42
SA Score	3.61
Color Est.	

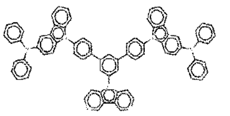


Nickname	november68-95
Splitting	0.118 (eV)
Strength	0.185
Absorption	2.68 (eV)
Rate	0.20 (1/ns)
HOMO	-4.74 (eV)
LUMO	-1.72 (eV)
Key	PFLQOVKCTNXJFT
Weight	1085.42
SA Score	3.77
Color Est.	

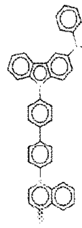


Nickname	november69-96
Splitting	0.077 (eV)
Strength	0.129
Absorption	2.65 (eV)
Rate	0.66 (1/ns)
HOMO	-4.67 (eV)
LUMO	-1.76 (eV)
Key	LJQLOVNIZQVVCW
Weight	869.34
SA Score	2.83
Color Est.	

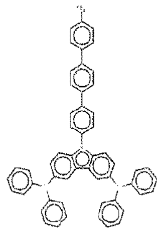
FIGURE 33



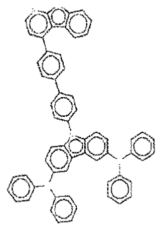
Nickname	november70-97
Splitting	0.124 (eV)
Strength	0.152
Absorption	2.85 (eV)
Rate	0.15 (1 us)
HOMO	-4.79 (eV)
LUMO	-1.63 (eV)
Key	TZNQPLGCHDOPDS
Weight	1061.42
SA Score	3.61
Color Est.:	



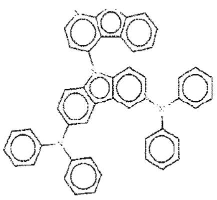
Nickname	november71-98
Splitting	0.168 (eV)
Strength	0.166
Absorption	2.98 (eV)
Rate	0.03 (1 us)
HOMO	-4.83 (eV)
LUMO	-1.53 (eV)
Key	BWGPBUNOCGVNLW
Weight	629.25
SA Score	2.64
Color Est.:	



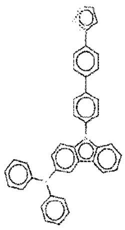
Nickname	november72-99
Splitting	0.132 (eV)
Strength	0.184
Absorption	2.80 (eV)
Rate	0.13 (1 us)
HOMO	-4.67 (eV)
LUMO	-1.58 (eV)
Key	XHVZORLQMOWKEN
Weight	797.30
SA Score	2.72
Color Est.:	



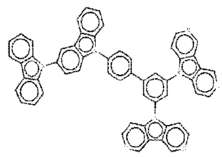
Nickname	november73-100
Splitting	0.105 (eV)
Strength	0.144
Absorption	2.80 (eV)
Rate	0.28 (1 us)
HOMO	-4.67 (eV)
LUMO	-1.59 (eV)
Key	HOESPCYVJGPLNW
Weight	836.30
SA Score	3.12
Color Est.:	



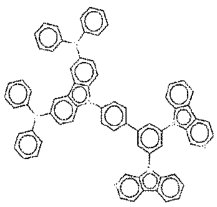
Nickname	november73-101
Splitting	0.077 (eV)
Strength	0.055
Absorption	2.74 (eV)
Rate	0.30 (1 us)
HOMO	-4.76 (eV)
LUMO	-1.57 (eV)
Key	PFTCYVCXBUANCU
Weight	684.23
SA Score	2.88
Color Est.:	



Nickname	november74-102
Splitting	0.142 (eV)
Strength	0.104
Absorption	2.74 (eV)
Rate	0.05 (1 us)
HOMO	-4.75 (eV)
LUMO	-1.71 (eV)
Key	KQOBNDLEOXPRBR
Weight	553.22
SA Score	2.55
Color Est.:	

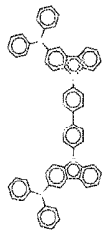


Nickname	november75-103
Splitting	0.149 (eV)
Strength	0.090
Absorption	3.05 (eV)
Rate	0.04 (1 us)
HOMO	-5.29 (eV)
LUMO	-1.93 (eV)
Key	PRVLOOBNAFGYLZ
Weight	818.29
SA Score	3.18
Color Est.:	

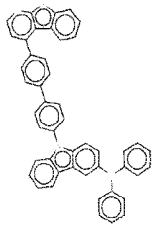


Nickname	november76-104
Splitting	0.149 (eV)
Strength	0.206
Absorption	2.80 (eV)
Rate	0.07 (1 us)
HOMO	-4.67 (eV)
LUMO	-1.53 (eV)
Key	VNVNCBSCIPLCKX
Weight	985.39
SA Score	3.48
Color Est.:	

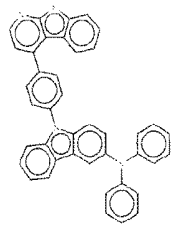
FIGURE 34



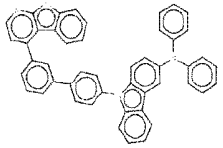
Nickname	november77-105
Splitting	0.174 (eV)
Strength	0.311
Absorption	2.65 (eV)
Rate	0.04 (1/ns)
HOMO	-4.79 (eV)
LUMO	-1.77 (eV)
Key	RJFJCAJQCQVUCW
Weight	870.33
SA Score	2.94
Color Est.	



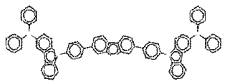
Nickname	november78-106
Splitting	0.103 (eV)
Strength	0.103
Absorption	2.86 (eV)
Rate	0.22 (1/ns)
HOMO	-4.76 (eV)
LUMO	-1.63 (eV)
Key	IVZMZAWBYGNNNJZ
Weight	669.22
SA Score	2.81
Color Est.	



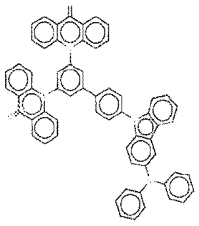
Nickname	november78-107
Splitting	0.036 (eV)
Strength	0.081
Absorption	2.91 (eV)
Rate	0.24 (1/ns)
HOMO	-4.79 (eV)
LUMO	-1.87 (eV)
Key	SHHFWJOCBUHHSC
Weight	593.49
SA Score	2.67
Color Est.	



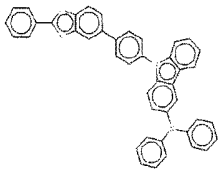
Nickname	november78-108
Splitting	0.121 (eV)
Strength	0.051
Absorption	3.01 (eV)
Rate	0.06 (1/ns)
HOMO	-4.75 (eV)
LUMO	-1.49 (eV)
Key	MDDJMWQNUOAPG
Weight	669.22
SA Score	2.84
Color Est.	



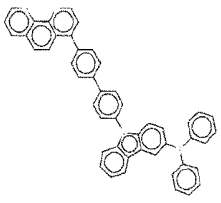
Nickname	november79-109
Splitting	0.171 (eV)
Strength	0.313
Absorption	2.79 (eV)
Rate	0.05 (1/ns)
HOMO	-4.72 (eV)
LUMO	-1.65 (eV)
Key	HNUDHAJORCMBF
Weight	1010.36
SA Score	3.29
Color Est.	



Nickname	november80-110
Splitting	0.113 (eV)
Strength	0.436
Absorption	2.73 (eV)
Rate	0.19 (1/ns)
HOMO	-4.87 (eV)
LUMO	-1.81 (eV)
Key	UWLMSCAQRHFUQX
Weight	872.32
SA Score	3.03
Color Est.	

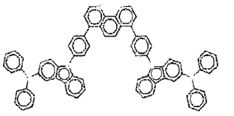


Nickname	november81-111
Splitting	0.133 (eV)
Strength	0.086
Absorption	2.66 (eV)
Rate	0.05 (1/ns)
HOMO	-4.71 (eV)
LUMO	-1.89 (eV)
Key	ZRMRIVCVOYEOOL
Weight	619.21
SA Score	2.58
Color Est.	

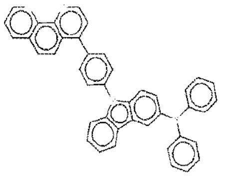


Nickname	november83-113
Splitting	0.122 (eV)
Strength	0.095
Absorption	2.86 (eV)
Rate	0.10 (1/ns)
HOMO	-4.74 (eV)
LUMO	-1.63 (eV)
Key	UBIPCRWHLITEHG
Weight	664.26
SA Score	2.81
Color Est.	

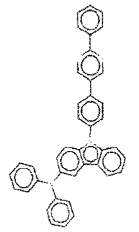
FIGURE 35



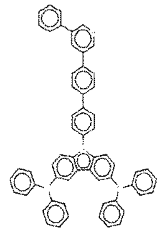
Nickname	november83-114
Splitting	0.115 (eV)
Strength	0.079
Absorption	2.82 (eV)
Rate	0.11 (1 us)
HOMO	-4.79 (eV)
LUMO	-1.70 (eV)
Key	VKYASEJWBRFDRU
Weight	996.39
SA Score	3.40
Color Est.:	



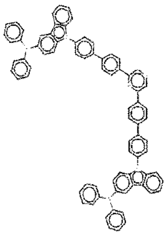
Nickname	november83-115
Splitting	0.129 (eV)
Strength	0.068
Absorption	2.87 (eV)
Rate	0.05 (1 us)
HOMO	-4.78 (eV)
LUMO	-1.61 (eV)
Key	IWSQWTDYDNDKNQ
Weight	588.23
SA Score	2.65
Color Est.:	



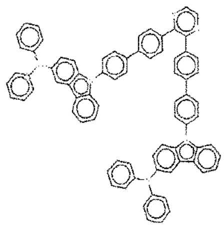
Nickname	november84-116
Splitting	0.108 (eV)
Strength	0.112
Absorption	2.74 (eV)
Rate	0.18 (1 us)
HOMO	-4.78 (eV)
LUMO	-1.74 (eV)
Key	VVQIVBTZPUGCBC
Weight	564.23
SA Score	2.46
Color Est.:	



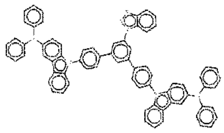
Nickname	november85-117
Splitting	0.166 (eV)
Strength	0.206
Absorption	2.87 (eV)
Rate	0.04 (1 us)
HOMO	-4.64 (eV)
LUMO	-1.46 (eV)
Key	ZPHJPBXASRDROU
Weight	806.34
SA Score	2.77
Color Est.:	



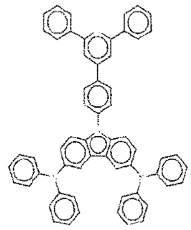
Nickname	november86-118
Splitting	0.082 (eV)
Strength	0.168
Absorption	2.67 (eV)
Rate	0.71 (1 us)
HOMO	-4.74 (eV)
LUMO	-1.83 (eV)
Key	RYPFQDBZZJINOOK
Weight	1048.43
SA Score	3.39
Color Est.:	



Nickname	november86-119
Splitting	0.116 (eV)
Strength	0.120
Absorption	2.72 (eV)
Rate	0.14 (1 us)
HOMO	-4.72 (eV)
LUMO	-1.74 (eV)
Key	NTLZOYQZGIWYIY
Weight	1048.43
SA Score	3.37
Color Est.:	

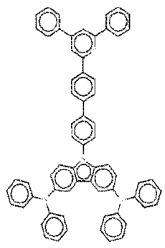


Nickname	november87-120
Splitting	0.123 (eV)
Strength	0.167
Absorption	2.92 (eV)
Rate	0.18 (1 us)
HOMO	-4.73 (eV)
LUMO	-1.53 (eV)
Key	RRXHZLIRTWDQRS
Weight	1011.40
SA Score	3.45
Color Est.:	

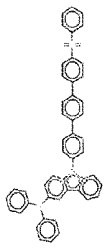


Nickname	november88-121
Splitting	0.154 (eV)
Strength	0.182
Absorption	2.81 (eV)
Rate	0.12 (1 us)
HOMO	-4.67 (eV)
LUMO	-1.54 (eV)
Key	PUOATUUYVBDSQC
Weight	806.34
SA Score	2.78
Color Est.:	

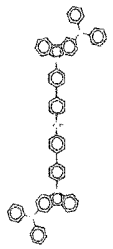
FIGURE 36



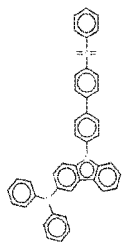
Nickname	november88-122
Splitting	0.146 (eV)
Strength	0.181
Absorption	2.82 (eV)
Rate	0.07 (1/ns)
HOMO	-4.61 (eV)
LUMO	-1.53 (eV)
Key	UDGRONARDZFAFQ
Weight	882.37
SA Score	2.91
Color Est.	



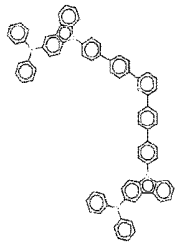
Nickname	november89-123
Splitting	0.095 (eV)
Strength	0.111
Absorption	2.74 (eV)
Rate	0.31 (1/ns)
HOMO	-4.75 (eV)
LUMO	-1.76 (eV)
Key	ILDPTAWFMPPCV
Weight	702.23
SA Score	2.52
Color Est.	



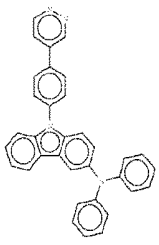
Nickname	november90-124
Splitting	0.063 (eV)
Strength	0.156
Absorption	2.67 (eV)
Rate	1.37 (1/ns)
HOMO	-4.78 (eV)
LUMO	-1.85 (eV)
Key	HRJZLJXAMAEHEE
Weight	1034.37
SA Score	3.23
Color Est.	



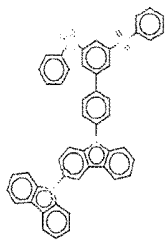
Nickname	november91-125
Splitting	0.107 (eV)
Strength	0.117
Absorption	2.76 (eV)
Rate	0.20 (1/ns)
HOMO	-4.80 (eV)
LUMO	-1.71 (eV)
Key	QDCVCIOVDBYMSV
Weight	626.20
SA Score	2.43
Color Est.	



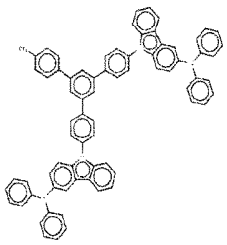
Nickname	november91-126
Splitting	0.166 (eV)
Strength	0.177
Absorption	2.88 (eV)
Rate	0.03 (1/ns)
HOMO	-4.70 (eV)
LUMO	-1.54 (eV)
Key	LSXJVTCINLASRF
Weight	1047.43
SA Score	3.31
Color Est.	



Nickname	november92-127
Splitting	0.113 (eV)
Strength	0.099
Absorption	2.66 (eV)
Rate	0.13 (1/ns)
HOMO	-4.84 (eV)
LUMO	-1.84 (eV)
Key	ZQLWHAMVLAH
Weight	488.20
SA Score	2.44
Color Est.	

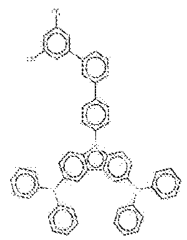
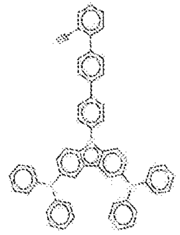
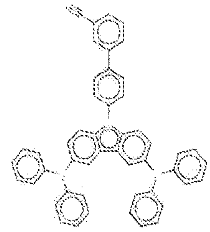
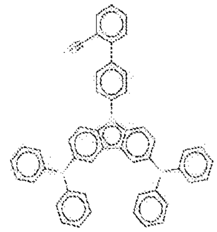


Nickname	november93-128
Splitting	0.150 (eV)
Strength	0.070
Absorption	3.05 (eV)
Rate	0.03 (1/ns)
HOMO	-5.22 (eV)
LUMO	-1.89 (eV)
Key	AQEQMBJLJPUGR
Weight	764.18
SA Score	2.66
Color Est.	

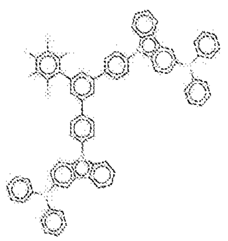
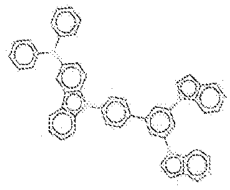
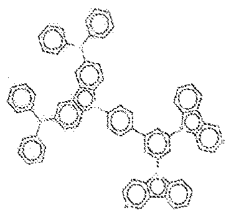
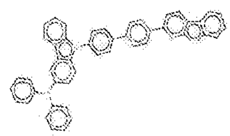


Nickname	november94-129
Splitting	0.160 (eV)
Strength	0.153
Absorption	3.00 (eV)
Rate	0.04 (1/ns)
HOMO	-4.76 (eV)
LUMO	-1.49 (eV)
Key	QWVFUFCDWFRFRG
Weight	1088.35
SA Score	3.35
Color Est.	

FIGURE 37

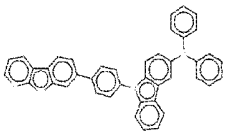





Nickname	november95-130	november96-131	november96-132	november96-133
Splitting	0.059 (eV)	0.084 (eV)	0.110 (eV)	0.090 (eV)
Strength	0.075	0.139	0.107	0.104
Absorption	2.85 (eV)	2.69 (eV)	2.77 (eV)	2.65 (eV)
Rate	0.19 (1/us)	0.47 (1/us)	0.50 (1/us)	0.53 (1/us)
HOMO	-4.67 (eV)	-4.62 (eV)	-4.71 (eV)	-4.62 (eV)
LUMO	-1.55 (eV)	-1.67 (eV)	-1.64 (eV)	-1.65 (eV)
Key	[illegible]	[illegible]	[illegible]	[illegible]
Weight	865.29	754.31	678.28	678.28
S.A Score	3.03	2.77	2.67	2.66
Color Est.:				

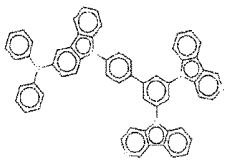





Nickname	november97-134	november98-135	november99-136	november100-137
Splitting	0.145 (eV)	0.158 (eV)	0.142 (eV)	0.128 (eV)
Strength	0.126	0.362	0.198	0.107
Absorption	2.97 (eV)	2.89 (eV)	2.75 (eV)	2.66 (eV)
Rate	0.06 (1/us)	0.08 (1/us)	0.09 (1/us)	0.08 (1/us)
HOMO	-4.77 (eV)	-4.83 (eV)	-4.75 (eV)	-4.59 (eV)
LUMO	-1.52 (eV)	-1.29 (eV)	-1.64 (eV)	-1.77 (eV)
Key	[illegible]	[illegible]	[illegible]	[illegible]
Weight	1060.36	718.28	985.30	675.25
S.A Score	3.40	3.19	3.46	2.78
Color Est.:				

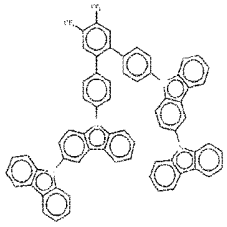
FIGURE 38



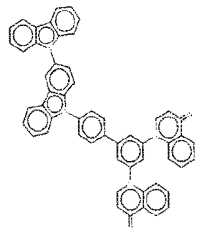
Nickname	[illegible]_Clone15_10-13
Splitting	0.142 (eV)
Strength	0.195
Absorption	2.81 (eV)
Rate	0.15 (1/ns)
HOMO	-4.73 (eV)
LUMO	-1.65 (eV)
Key	QUGBNFZHYUAFFO
Weight	577.22
SA Score	2.67
Color Est.	



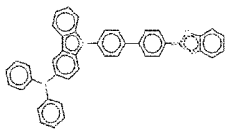
Nickname	november101-139
Splitting	0.147 (eV)
Strength	0.145
Absorption	2.88 (eV)
Rate	0.06 (1/ns)
HOMO	-4.84 (eV)
LUMO	-1.62 (eV)
Key	VZOXTPSYRMBAHY
Weight	818.32
SA Score	3.14
Color Est.	



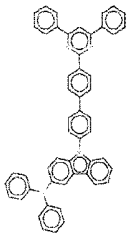
Nickname	november102-140
Splitting	0.124 (eV)
Strength	0.079
Absorption	3.03 (eV)
Rate	0.09 (1/ns)
HOMO	-5.27 (eV)
LUMO	-1.95 (eV)
Key	TYEPFXNNYCSPHB
Weight	1026.32
SA Score	3.26
Color Est.	



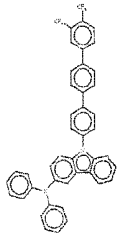
Nickname	november103-141
Splitting	0.148 (eV)
Strength	0.098
Absorption	3.03 (eV)
Rate	0.04 (1/ns)
HOMO	-5.30 (eV)
LUMO	-1.96 (eV)
Key	LGASRKWTXZHNG
Weight	770.27
SA Score	2.98
Color Est.	



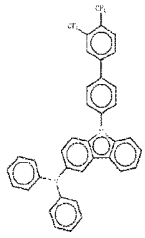
Nickname	november104-142
Splitting	0.121 (eV)
Strength	0.110
Absorption	2.69 (eV)
Rate	0.11 (1/ns)
HOMO	-4.73 (eV)
LUMO	-1.76 (eV)
Key	URRXFMRFXMAVJV
Weight	663.23
SA Score	2.56
Color Est.	



Nickname	november105-143
Splitting	0.115 (eV)
Strength	0.092
Absorption	2.76 (eV)
Rate	0.12 (1/ns)
HOMO	-4.67 (eV)
LUMO	-4.71 (eV)
Key	ZXTMRRLDMGMHK7
Weight	716.29
SA Score	2.64
Color Est.	

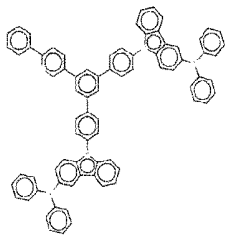


Nickname	november106-144
Splitting	0.080 (eV)
Strength	0.097
Absorption	2.70 (eV)
Rate	0.46 (1/ns)
HOMO	-4.79 (eV)
LUMO	-1.83 (eV)
Key	BVUTWZCHOLLBSG
Weight	698.22
SA Score	2.71
Color Est.	

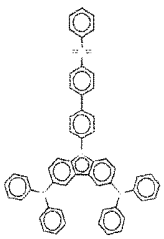


Nickname	november106-145
Splitting	0.091 (eV)
Strength	0.089
Absorption	2.71 (eV)
Rate	0.27 (1/ns)
HOMO	-4.83 (eV)
LUMO	-1.80 (eV)
Key	RPVCRYYDDQCNQJ
Weight	622.18
SA Score	2.65
Color Est.	

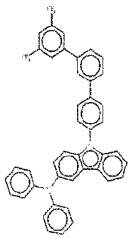
FIGURE 39



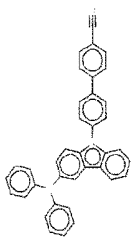
Nickname	november107-146
Splitting	0.153 (eV)
Strength	0.057
Absorption	2.96 (eV)
Rate	0.02 (1/ns)
HOMO	-4.75 (eV)
LUMO	-1.55 (eV)
Key	VOXDNBOLSQFQFJ
Weight	1047.48
SA Score	3.44
Color Est.	



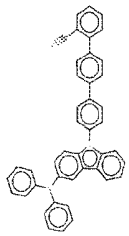
Nickname	november108-147
Splitting	0.107 (eV)
Strength	0.161
Absorption	3.67 (eV)
Rate	0.26 (1/ns)
HOMO	-4.71 (eV)
LUMO	-1.73 (eV)
Key	WHVINCQVSLAQSD
Weight	793.28
SA Score	2.71
Color Est.	



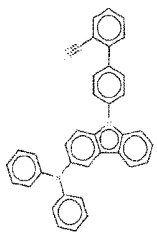
Nickname	november109-148
Splitting	0.149 (eV)
Strength	0.063
Absorption	2.96 (eV)
Rate	0.08 (1/ns)
HOMO	-4.76 (eV)
LUMO	-1.53 (eV)
Key	UKXMFRARMKJCAB
Weight	698.22
SA Score	2.75
Color Est.	



Nickname	november110-149
Splitting	0.096 (eV)
Strength	0.099
Absorption	2.66 (eV)
Rate	0.25 (1/ns)
HOMO	-4.82 (eV)
LUMO	-1.86 (eV)
Key	XGWNOZCATGOFTS
Weight	511.20
SA Score	2.44
Color Est.	



Nickname	november110-150
Splitting	0.084 (eV)
Strength	0.084
Absorption	2.78 (eV)
Rate	0.36 (1/ns)
HOMO	-4.71 (eV)
LUMO	-1.68 (eV)
Key	QUTCMVHYMYFNG
Weight	587.24
SA Score	2.50
Color Est.	



Nickname	november110-151
Splitting	0.099 (eV)
Strength	0.080
Absorption	2.78 (eV)
Rate	0.27 (1/ns)
HOMO	-4.75 (eV)
LUMO	-1.65 (eV)
Key	LYHHAILGSIPVKA
Weight	511.20
SA Score	2.37
Color Est.	

FIGURE 40

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_1-1	0.115	0.164	2.64	0.19	-5.35	-2.46	SFTLTAIATUCOTA	975.3	3.7
		malika_June15_2-2	0.094	0.345	2.37	0.72	-4.81	-2.16	ZSEKHCGCECHRSS	977.3	3.5
		malika_June15_3-3	0.082	0.065	2.45	0.24	-4.81	-2.12	OYVZZYDDHHWQGY	614.2	2.6
		malika_June15_4-4	0.108	0.112	2.49	0.15	-4.77	-2.04	PTDFELQUSUKYKL	857.4	3.1
		malika_June15_5-5	0.086	0.289	2.24	0.75	-4.94	-2.43	RZUADAGPASJKKJ	979.3	3.8
		malika_June15_6-6	0.107	0.193	2.54	0.28	-4.76	-1.96	UQGGWWRCVHRUIA	960.4	3.0
		malika_June15_7-10	0.047	0.067	2.31	0.79	-4.87	-2.33	GWUIHOCUORHTBY	858.3	3.1

Table 3

FIGURE 41

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_7-7	0.145	0.173	2.30	0.05	-4.73	-2.20	KISCHLHCSIQVFW	934.4	3.3
		malika_June15_7-8	0.075	0.093	2.46	0.44	-4.81	-2.21	KPGHGOUURLFUGR	1010.4	3.4
		malika_June15_7-11	0.053	0.067	2.09	0.53	-4.71	-2.39	FSWSBLRTMGGADK	858.3	3.2
		malika_June15_7-9	0.128	0.076	2.03	0.03	-4.73	-2.39	HYXSTDHRAOIUCF	782.3	3.0
		malika_June15_8-12	0.119	0.129	2.76	0.14	-4.82	-1.81	QASSHQGCNNWWFU	716.3	2.6
		malika_June15_9-13	0.147	0.055	3.01	0.02	-4.74	-1.44	QWQKUUIGWROEOF	592.3	2.7
		malika_June15_9-14	0.082	0.052	2.89	0.26	-4.74	-1.55	HWWIADPRBZMXPC	592.3	2.7

FIGURE 42

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_10-16	0.046	0.052	2.78	0.93	-4.78	-1.74	ZMHGYRUOJNYUJO	897.4	3.1
		malika_June15_10-15	0.060	0.061	2.88	0.68	-4.78	-1.66	IPKFMOMFBQSZOG	911.4	3.2
		malika_June15_11-17	0.090	0.261	2.30	0.62	-4.73	-2.17	FEQPWGZKBPAQLG	986.4	3.5
		malika_June15_12-18	0.097	0.360	2.34	0.67	-4.81	-2.19	HDBAKJAVFHSWHJ	1009.3	3.5
		malika_June15_13-19	0.074	0.110	2.48	0.54	-4.79	-2.10	JYAYHCGUXIJOMD	965.4	3.2
		malika_June15_14-20	0.073	0.271	2.36	1.25	-4.94	-2.31	YDUBECAOCYWOH	979.3	3.7
		malika_June15_15-21	0.114	0.369	2.24	0.32	-4.80	-2.29	AQACLJKKDPLQQT	977.3	3.6

FIGURE 43

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_16-22	0.123	0.183	2.59	0.15	-4.66	-1.78	KMURVOKKIYSPDO	770.3	2.8
		malika_June15_17-23	0.102	0.079	2.88	0.18	-4.79	-1.71	FMWIODAUSGIBFG	806.3	3.0
		malika_June15_18-24	0.114	0.062	2.94	0.09	-4.76	-1.60	FANYFEJLSAYDMZ	654.3	2.7
		malika_June15_19-25	0.084	0.132	2.51	0.46	-4.86	-2.11	UFSIYRVQGLVGAD	1009.3	3.3
		malika_June15_20-26	0.103	0.386	2.34	0.56	-4.81	-2.20	BBNMYUAGEASBEE	977.3	3.5
		malika_June15_21-27	0.144	0.321	2.63	0.12	-4.81	-1.93	OGAZXLKSAPZPFQ	1048.4	3.3
		malika_June15_22-28	0.126	0.141	1.82	0.05	-4.95	-2.90	BIFSMPUPEASBAG	805.3	3.0

FIGURE 44

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_23-29	0.134	0.417	2.56	0.22	-4.79	-1.94	FULHEGOGYLWNQU	976.4	3.4
		malika_June15_24-31	0.048	0.088	2.18	0.92	-4.88	-2.48	XDEBWBHDSOIXFH	855.3	3.0
		malika_June15_24-30	0.108	0.092	2.31	0.11	-4.98	-2.39	DWCCSOQMELEXGO	779.3	2.9
		malika_June15_24-34	0.019	0.052	2.20	1.51	-4.84	-2.46	YITMHPZCJDIOHO	931.4	3.1
		malika_June15_24-33	0.116	0.072	2.38	0.07	-4.85	-2.30	HVKQSQGGGLYJRR	931.4	3.1
		malika_June15_24-32	0.053	0.082	2.34	0.79	-4.83	-2.35	BLHAANDCAHEINV	1007.4	3.2
		malika_June15_26-36	0.148	0.151	2.64	0.05	-4.70	-1.76	JTWSGVZQOZOHLT	577.2	2.6

FIGURE 45

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_27-38	0.076	0.212	2.30	0.83	-4.88	-2.32	SGKVTECHUIMQHK	988.4	3.7
		malika_June15_28-39	0.136	0.131	2.29	0.05	-4.88	-2.34	JSGCIQCFPCOJOD	825.3	2.9
		malika_June15_28-40	0.020	0.050	2.24	1.47	-4.80	-2.38	WQRFYBUPRWLDNL	977.4	3.2
		malika_June15_29-42	0.037	0.108	2.02	1.39	-4.88	-2.67	LKCWZXKTUCTFGZ	789.3	3.0
		malika_June15_29-41	0.111	0.203	2.09	0.18	-4.97	-2.63	VRGCFYMCSRIURD	713.3	2.9
		malika_June15_30-43	0.073	0.268	2.33	1.20	-4.95	-2.36	VMHKKWPKMUMVOY	979.3	3.7
		malika_June15_31-44	0.148	0.319	2.45	0.09	-4.93	-2.20	XXODHIKABBLARM	978.3	3.6

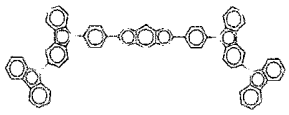
FIGURE 46

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_32-45	0.096	0.305	2.54	0.69	-4.93	-2.10	UGDSJSIIYCQWMI	978.3	3.6
		malika_June15_33-46	0.130	0.057	2.28	0.03	-4.84	-2.26	UDBBKTXWDHLRLJ	1050.4	3.7
		malika_June15_34-48	0.022	0.073	2.01	1.56	-4.81	-2.66	YGKTVZGRMCAZFV	1032.4	3.5
		malika_June15_34-47	0.041	0.085	1.84	0.80	-4.86	-2.79	EICFFCYPYZRXOG	880.3	3.2
		malika_June15_35-49	0.110	0.104	2.49	0.13	-4.72	-1.98	VJZNBIUPKHTZQM	857.4	3.0
		malika_June15_35-50	0.087	0.071	2.58	0.23	-4.73	-1.96	FZHYBRONXVUKEV	933.4	3.1
		malika_June15_35-51	0.079	0.055	2.60	0.25	-4.80	-1.98	VZFGIFBXJSTMAI	857.4	3.0

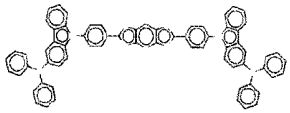
FIGURE 47

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		malika_June15_36-52	0.125	0.191	2.53	0.14	-4.59	-1.75	GLHBGRJFVYRGMN	744.3	3.0
		malika_June15_37-55	0.068	0.267	2.32	1.44	-4.94	-2.35	LJEXIGHVJZQWDQ	1011.3	3.7
		malika_June15_38-56	0.101	0.126	2.61	0.25	-4.81	-1.96	CTGCZGQYYXHILE	717.3	2.6
		malika_June15_39-57	0.119	0.228	1.94	0.12	-4.96	-2.81	YKYWBVATDBFPBS	714.3	2.8

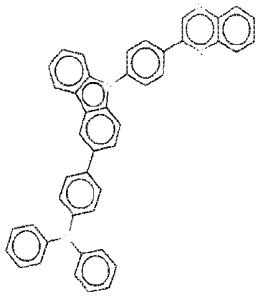
FIGURE 48



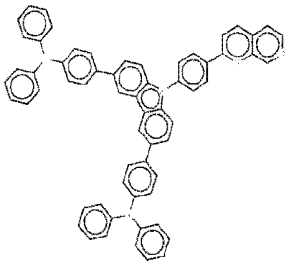
Nickname	malika_June15_1-1
Splitting	0.115 (eV)
Strength	0.164
Absorption	2.64 (eV)
Rate	0.19 (1/fs)
HOMO	-5.35 (eV)
LUMO	-2.46 (eV)
Key	SFTLEAATUOOTA
Weight	975.31
SA Score	3.65
Color Est.:	



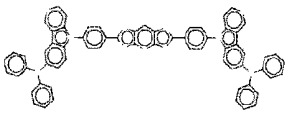
Nickname	malika_June15_2-2
Splitting	0.094 (eV)
Strength	0.345
Absorption	2.37 (eV)
Rate	0.72 (1/fs)
HOMO	-4.81 (eV)
LUMO	-2.16 (eV)
Key	ZSERCIOGCECTHRSS
Weight	977.35
SA Score	3.50
Color Est.:	



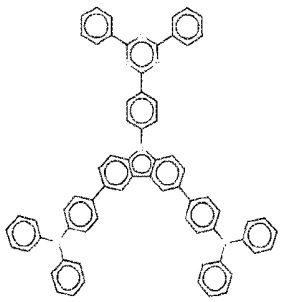
Nickname	malika_June15_3-3
Splitting	0.082 (eV)
Strength	0.065
Absorption	2.45 (eV)
Rate	0.24 (1/fs)
HOMO	-4.81 (eV)
LUMO	-2.12 (eV)
Key	OYVZZYIDBHWQGY
Weight	614.25
SA Score	2.57
Color Est.:	



Nickname	malika_June15_4-4
Splitting	0.108 (eV)
Strength	0.112
Absorption	2.49 (eV)
Rate	0.15 (1/fs)
HOMO	-4.77 (eV)
LUMO	-2.04 (eV)
Key	PTDFFLQUSUKYKL
Weight	857.35
SA Score	3.10
Color Est.:	



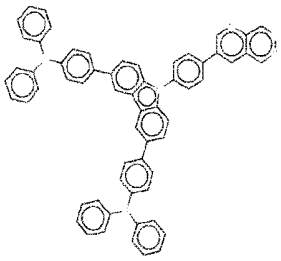
Nickname	malika_June15_5-5
Splitting	0.086 (eV)
Strength	0.289
Absorption	2.24 (eV)
Rate	0.75 (1/fs)
HOMO	-4.94 (eV)
LUMO	-2.43 (eV)
Key	RZTADAGPASIKKJ
Weight	979.34
SA Score	3.81
Color Est.:	



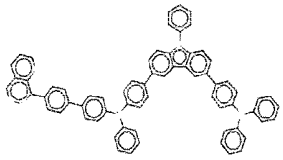
Nickname	malika_June15_6-6
Splitting	0.107 (eV)
Strength	0.193
Absorption	2.34 (eV)
Rate	0.28 (1/fs)
HOMO	-4.76 (eV)
LUMO	-1.96 (eV)
Key	UQGGWYRCVHRUIA
Weight	960.39
SA Score	3.04
Color Est.:	

Table 4

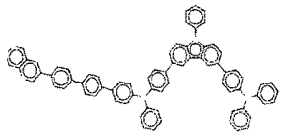
FIGURE 49



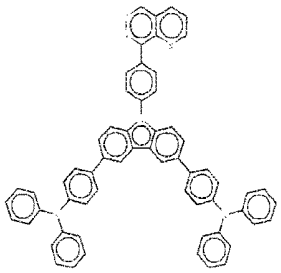
Nickname	malika_June15_7-10
Splitting	0.047 (eV)
Strength	0.067
Absorption	2.31 (eV)
Rate	0.79 (1/ns)
HOMO	-4.87 (eV)
LUMO	-2.33 (eV)
Key	GWTHOCVORHTBY
Weight	858.35
SA Score	3.13
Color Est.:	



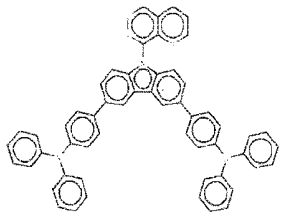
Nickname	malika_June15_7-7
Splitting	0.145 (eV)
Strength	0.173
Absorption	2.30 (eV)
Rate	0.65 (1/ns)
HOMO	-4.73 (eV)
LUMO	-2.29 (eV)
Key	KISCHLHCSRQVFW
Weight	934.38
SA Score	3.31
Color Est.:	



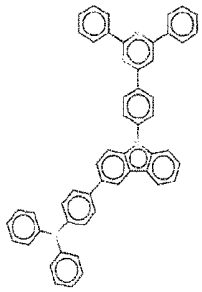
Nickname	malika_June15_7-8
Splitting	0.075 (eV)
Strength	0.093
Absorption	2.46 (eV)
Rate	0.44 (1/ns)
HOMO	-4.81 (eV)
LUMO	-2.21 (eV)
Key	KPGHGOUCRLFUGR
Weight	1010.41
SA Score	3.39
Color Est.:	



Nickname	malika_June15_7-11
Splitting	0.053 (eV)
Strength	0.067
Absorption	2.09 (eV)
Rate	0.53 (1/ns)
HOMO	-4.71 (eV)
LUMO	-2.39 (eV)
Key	FSWSBLRTMGBADK
Weight	858.35
SA Score	3.18
Color Est.:	

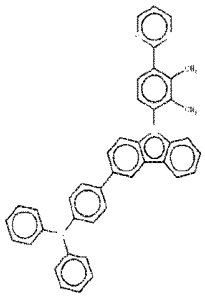


Nickname	malika_June15_7-9
Splitting	0.128 (eV)
Strength	0.976
Absorption	2.03 (eV)
Rate	0.03 (1/ns)
HOMO	-4.73 (eV)
LUMO	-2.39 (eV)
Key	HYNSTLDIRAORUCF
Weight	782.32
SA Score	3.03
Color Est.:	

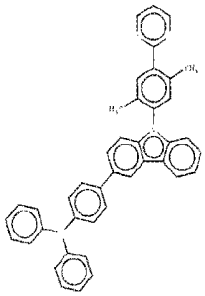


Nickname	malika_June15_8-12
Splitting	0.119 (eV)
Strength	0.129
Absorption	2.76 (eV)
Rate	0.14 (1/ns)
HOMO	-4.82 (eV)
LUMO	-1.81 (eV)
Key	QASSHQGCNNWWFV
Weight	716.29
SA Score	2.64
Color Est.:	

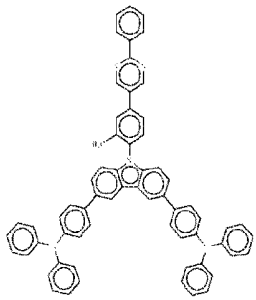
FIGURE 50



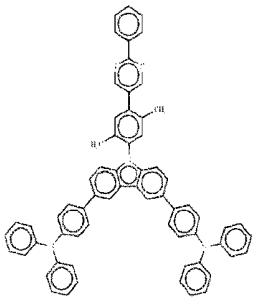
Nickname	malika_June15_9-13
Splitting	0.147 (eV)
Strength	0.055
Absorption	3.01 (eV)
Rate	0.02 (1/us)
HOMO	-4.74 (eV)
LUMO	-1.44 (eV)
Key	QWQKUCUGWROEOI-
Weight	592.26
SA Score	2.70
Color Est.	



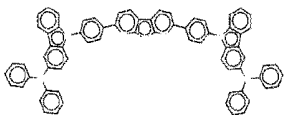
Nickname	malika_June15_9-14
Splitting	0.082 (eV)
Strength	0.052
Absorption	2.89 (eV)
Rate	0.26 (1/us)
HOMO	-4.74 (eV)
LUMO	-1.55 (eV)
Key	HWWLMDPRBZMIXPC
Weight	592.26
SA Score	2.69
Color Est.	



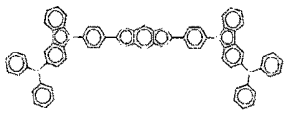
Nickname	malika_June15_10-16
Splitting	0.046 (eV)
Strength	0.052
Absorption	2.78 (eV)
Rate	0.93 (1/us)
HOMO	-4.78 (eV)
LUMO	-1.74 (eV)
Key	ZMHGYRVOJNYUJO
Weight	897.38
SA Score	3.00
Color Est.	



Nickname	malika_June15_10-15
Splitting	0.060 (eV)
Strength	0.061
Absorption	2.88 (eV)
Rate	0.68 (1/us)
HOMO	-4.78 (eV)
LUMO	-1.66 (eV)
Key	IPKFMOMFBQSZOG
Weight	911.40
SA Score	3.21
Color Est.	

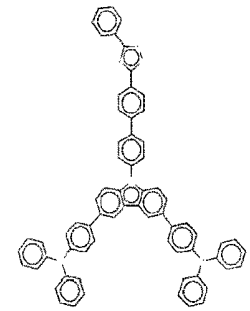


Nickname	malika_June15_11-17
Splitting	0.090 (eV)
Strength	0.261
Absorption	2.30 (eV)
Rate	0.62 (1/us)
HOMO	-4.73 (eV)
LUMO	-2.17 (eV)
Key	FEQPWGZKBPAQLG
Weight	986.37
SA Score	3.46
Color Est.	

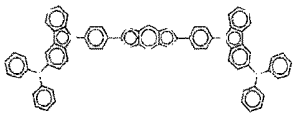


Nickname	malika_June15_12-18
Splitting	0.097 (eV)
Strength	0.360
Absorption	2.34 (eV)
Rate	0.67 (1/us)
HOMO	-4.81 (eV)
LUMO	-2.19 (eV)
Key	HDBAKIAVFHSWIH
Weight	1009.30
SA Score	3.48
Color Est.	

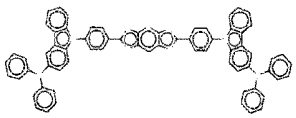
FIGURE 51



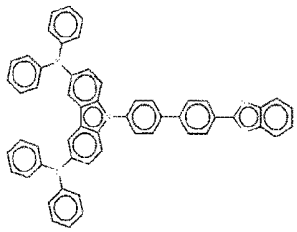
Nickname	malika_June15_13-19
Splitting	0.074 (eV)
Strength	0.110
Absorption	2.48 (eV)
Rate	0.54 (1/ns)
HOMO	-4.79 (eV)
LUMO	-2.10 (eV)
Key	JYAYHOGUXUOMD
Weight	965.36
SA Score	3.21
Color Est.	



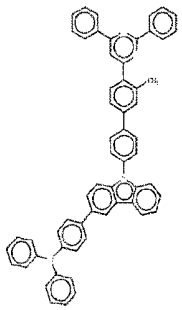
Nickname	malika_June15_14-20
Splitting	0.073 (eV)
Strength	0.271
Absorption	2.36 (eV)
Rate	1.25 (1/ns)
HOMO	-4.94 (eV)
LUMO	-2.31 (eV)
Key	YDUBECAOCYVIOH
Weight	979.34
SA Score	3.72
Color Est.	



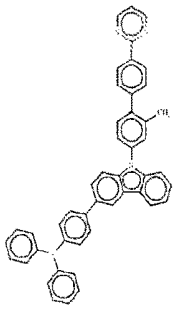
Nickname	malika_June15_15-21
Splitting	0.114 (eV)
Strength	0.369
Absorption	2.24 (eV)
Rate	0.32 (1/ns)
HOMO	-4.80 (eV)
LUMO	-2.29 (eV)
Key	AQACLJKKDPLQQT
Weight	977.35
SA Score	3.60
Color Est.	



Nickname	malika_June15_16-22
Splitting	0.123 (eV)
Strength	0.183
Absorption	2.59 (eV)
Rate	0.15 (1/ns)
HOMO	-4.66 (eV)
LUMO	-1.78 (eV)
Key	KMURVOKKIYSPDO
Weight	770.30
SA Score	2.85
Color Est.	

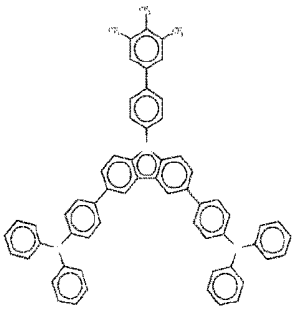


Nickname	malika_June15_17-23
Splitting	0.102 (eV)
Strength	0.079
Absorption	2.88 (eV)
Rate	0.18 (1/ns)
HOMO	-4.79 (eV)
LUMO	-1.71 (eV)
Key	FMWODAUSGIBHG
Weight	806.34
SA Score	2.96
Color Est.	

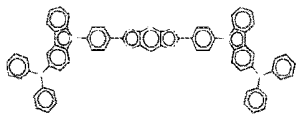


Nickname	malika_June15_18-24
Splitting	0.114 (eV)
Strength	0.062
Absorption	2.94 (eV)
Rate	0.09 (1/ns)
HOMO	-4.76 (eV)
LUMO	-1.60 (eV)
Key	FANYYEJLSAYDMZ
Weight	654.28
SA Score	2.73
Color Est.	

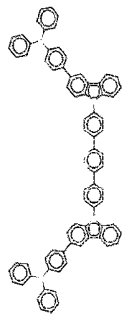
FIGURE 52



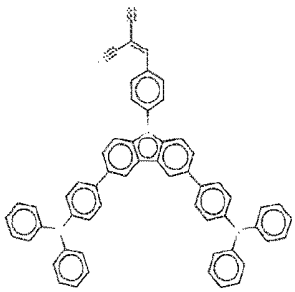
Nickname	malika_June15_19-25
Splitting	0.084 (eV)
Strength	0.132
Absorption	2.51 (eV)
Rate	0.46 (1/ns)
HOMO	-4.86 (eV)
LUMO	-2.11 (eV)
Key	UFSIYRVQGLVGAD
Weight	1000.31
SA Score	3.31
Color Est.	



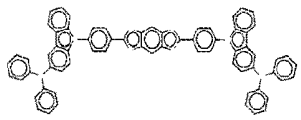
Nickname	malika_June15_20-26
Splitting	0.103 (eV)
Strength	0.386
Absorption	2.34 (eV)
Rate	0.56 (1/ns)
HOMO	-4.81 (eV)
LUMO	-2.20 (eV)
Key	BBNMYUAGEASBIE
Weight	977.35
SA Score	3.49
Color Est.	



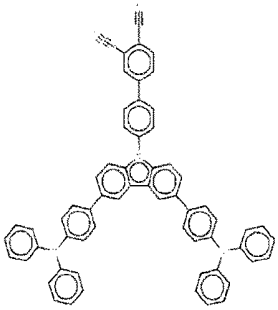
Nickname	malika_June15_21-27
Splitting	0.144 (eV)
Strength	0.321
Absorption	2.63 (eV)
Rate	0.12 (1/ns)
HOMO	-4.81 (eV)
LUMO	-1.93 (eV)
Key	OGAZXLKSAPZPFQ
Weight	1048.43
SA Score	3.31
Color Est.	



Nickname	malika_June15_22-28
Splitting	0.126 (eV)
Strength	0.141
Absorption	1.82 (eV)
Rate	0.05 (1/ns)
HOMO	-4.95 (eV)
LUMO	-2.90 (eV)
Key	BIFSMPUPEASBAG
Weight	805.32
SA Score	3.01
Color Est.	

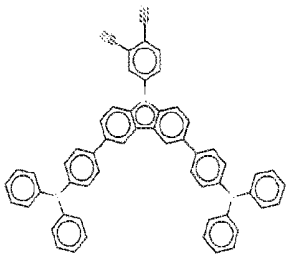


Nickname	malika_June15_23-29
Splitting	0.134 (eV)
Strength	0.417
Absorption	2.56 (eV)
Rate	0.22 (1/ns)
HOMO	-4.79 (eV)
LUMO	-1.94 (eV)
Key	FUUIEGOGVLWNQU
Weight	976.35
SA Score	3.41
Color Est.	

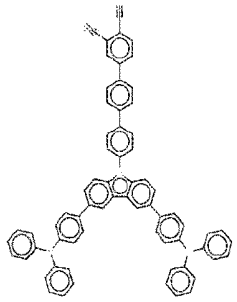


Nickname	malika_June15_24-31
Splitting	0.048 (eV)
Strength	0.088
Absorption	2.38 (eV)
Rate	0.92 (1/ns)
HOMO	-4.88 (eV)
LUMO	-2.48 (eV)
Key	NDEBWBHDSOINFH
Weight	835.34
SA Score	2.98
Color Est.	

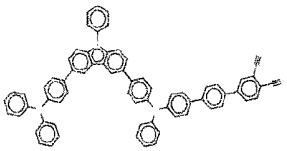
FIGURE 53



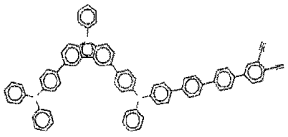
Nickname	malika_June15_24-30
Splitting	0.108 (eV)
Strength	0.092
Absorption	2.31 (eV)
Rate	0.13 (1/fs)
HOMO	-4.98 (eV)
LUMO	-2.39 (eV)
Key	DWCUSOQAIELEXG-G
Weight	779.36
SA Score	2.87
Color Est.:	



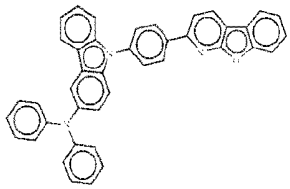
Nickname	malika_June15_24-34
Splitting	0.019 (eV)
Strength	0.052
Absorption	2.20 (eV)
Rate	1.51 (1/fs)
HOMO	-4.84 (eV)
LUMO	-2.46 (eV)
Key	YITMHPZCJDIOHE-UHFFFAOYSA-N
Weight	931.37
SA Score	3.11
Color Est.:	



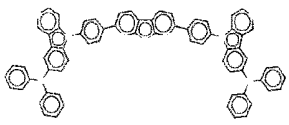
Nickname	malika_June15_24-33
Splitting	0.116 (eV)
Strength	0.072
Absorption	2.38 (eV)
Rate	0.07 (1/fs)
HOMO	-4.85 (eV)
LUMO	-2.30 (eV)
Key	HVKQSQQGGHYJRR-UHFFFAOYSA-N
Weight	931.37
SA Score	3.11
Color Est.:	



Nickname	malika_June15_24-32
Splitting	0.053 (eV)
Strength	0.082
Absorption	2.34 (eV)
Rate	0.79 (1/fs)
HOMO	-4.83 (eV)
LUMO	-2.35 (eV)
Key	BLHAANDCAHHENV-UHFFFAOYSA-N
Weight	1007.40
SA Score	3.25
Color Est.:	

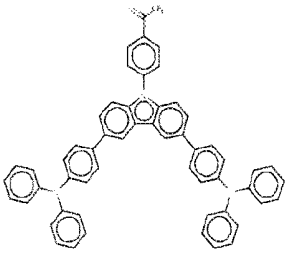


Nickname	malika_June15_26-36
Splitting	0.148 (eV)
Strength	0.151
Absorption	2.64 (eV)
Rate	0.05 (1/fs)
HOMO	-4.70 (eV)
LUMO	-1.76 (eV)
Key	JTWSGWZQCSZOHB-UHFFFAOYSA-T
Weight	577.22
SA Score	2.63
Color Est.:	

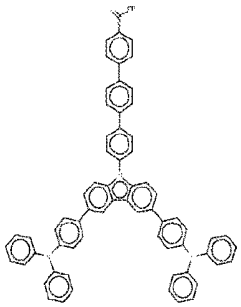


Nickname	malika_June15_27-38
Splitting	0.076 (eV)
Strength	0.212
Absorption	2.30 (eV)
Rate	0.83 (1/fs)
HOMO	-4.88 (eV)
LUMO	-2.32 (eV)
Key	SGKVTBGHUTMQHK-UHFFFAOYSA-N
Weight	988.36
SA Score	3.67
Color Est.:	

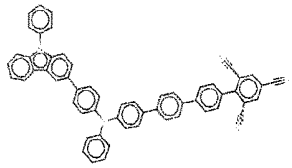
FIGURE 54



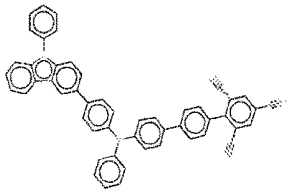
Nickname	malika_June15_28-39
Splitting	0.136 (eV)
Strength	0.431
Absorption	2.29 (eV)
Rate	0.05 (1/ns)
HOMO	-4.88 (eV)
LUMO	-2.34 (eV)
Key	JSGCIQCIPCDJOD
Weight	825.30
SA Score	2.90
Color Est.:	



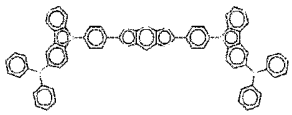
Nickname	malika_June15_28-40
Splitting	0.020 (eV)
Strength	0.050
Absorption	2.24 (eV)
Rate	1.47 (1/ns)
HOMO	-4.80 (eV)
LUMO	-2.38 (eV)
Key	WQRFVBUPRWLDNL
Weight	977.36
SA Score	3.16
Color Est.:	



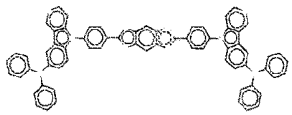
Nickname	malika_June15_29-42
Splitting	0.037 (eV)
Strength	0.108
Absorption	2.92 (eV)
Rate	1.39 (1/ns)
HOMO	-4.88 (eV)
LUMO	-2.67 (eV)
Key	LKCWZXKTUTTFGZ
Weight	789.29
SA Score	3.04
Color Est.:	



Nickname	malika_June15_29-41
Splitting	0.111 (eV)
Strength	0.203
Absorption	2.99 (eV)
Rate	0.18 (1/ns)
HOMO	-4.97 (eV)
LUMO	-2.63 (eV)
Key	VRGCFYMCSRUCRD
Weight	713.26
SA Score	2.95
Color Est.:	

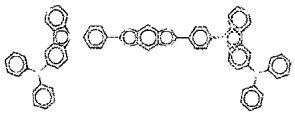


Nickname	malika_June15_30-43
Splitting	0.073 (eV)
Strength	0.268
Absorption	2.33 (eV)
Rate	1.30 (1/ns)
HOMO	-4.95 (eV)
LUMO	-2.36 (eV)
Key	VMHKKWPRMUMVOY
Weight	979.34
SA Score	3.71
Color Est.:	

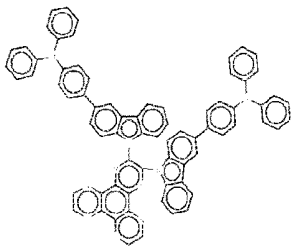


Nickname	malika_June15_31-44
Splitting	0.148 (eV)
Strength	0.319
Absorption	2.45 (eV)
Rate	0.09 (1/ns)
HOMO	-4.93 (eV)
LUMO	-2.20 (eV)
Key	XXODHKABBLARM
Weight	978.34
SA Score	3.62
Color Est.:	

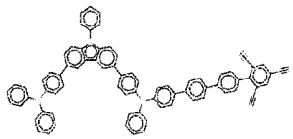
FIGURE 55



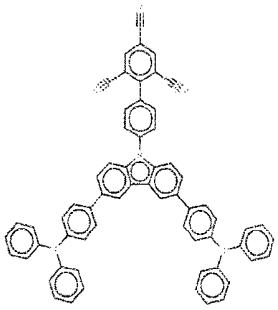
Nickname	malika_June15_32-45
Splitting	0.026 (eV)
Strength	0.305
Absorption	2.54 (eV)
Rate	0.69 (1/ns)
HOMO	-4.93 (eV)
LUMO	-2.10 (eV)
Key	UGDSISHYCQAWMI
Weight	978.34
SA Score	3.62
Color Est.	



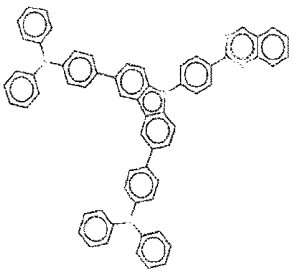
Nickname	malika_June15_33-46
Splitting	0.130 (eV)
Strength	0.057
Absorption	2.28 (eV)
Rate	0.03 (1/ns)
HOMO	-4.84 (eV)
LUMO	-2.26 (eV)
Key	UDHBXTXWDHLRLJ
Weight	1050.39
SA Score	3.68
Color Est.	



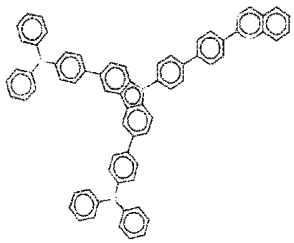
Nickname	malika_June15_34-48
Splitting	0.022 (eV)
Strength	0.073
Absorption	2.01 (eV)
Rate	1.56 (1/ns)
HOMO	-4.81 (eV)
LUMO	-2.66 (eV)
Key	YGKTVZGRMCAZFV
Weight	1032.39
SA Score	3.48
Color Est.	



Nickname	malika_June15_34-47
Splitting	0.041 (eV)
Strength	0.085
Absorption	1.84 (eV)
Rate	0.80 (1/ns)
HOMO	-4.86 (eV)
LUMO	-2.79 (eV)
Key	BICHFCYPYZRXOG
Weight	880.33
SA Score	3.22
Color Est.	

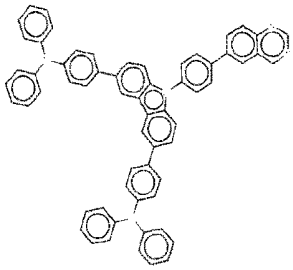


Nickname	malika_June15_35-49
Splitting	0.110 (eV)
Strength	0.104
Absorption	2.49 (eV)
Rate	0.13 (1/ns)
HOMO	-4.72 (eV)
LUMO	-1.98 (eV)
Key	VJZNBIUPKHTZQM
Weight	857.45
SA Score	3.91
Color Est.	

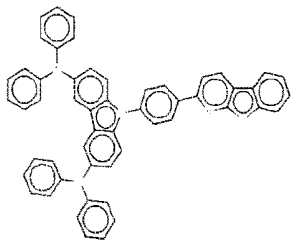


Nickname	malika_June15_35-50
Splitting	0.087 (eV)
Strength	0.071
Absorption	2.58 (eV)
Rate	0.23 (1/ns)
HOMO	-4.73 (eV)
LUMO	-1.96 (eV)
Key	FZHYBHOSXVUKEV
Weight	935.38
SA Score	3.15
Color Est.	

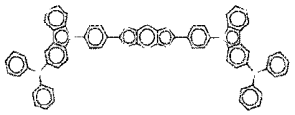
FIGURE 56



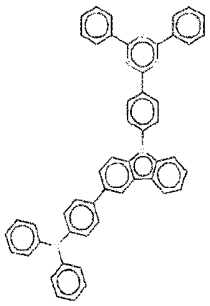
Nickname	malika_June15_35-51
Splitting	0.079 (eV)
Strength	0.055
Absorption	2.60 (eV)
Rate	0.25 (1/fs)
HOMO	-4.80 (eV)
LUMO	-1.98 (eV)
Key	VZBGBFBXJSTMAI
Weight	857.35
SA Score	4.03
Color Est.	



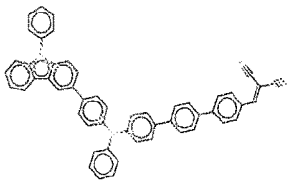
Nicknamc	malika_June15_36-52
Splitting	0.125 (eV)
Strength	0.191
Absorption	2.53 (eV)
Rate	0.14 (1/fs)
HOMO	-4.59 (eV)
LUMO	-1.75 (eV)
Key	GLHBGRJFVYRGMN
Weight	744.29
SA Score	2.96
Color Est.	



Nicknamc	malika_June15_37-55
Splitting	0.068 (eV)
Strength	0.267
Absorption	2.32 (eV)
Rate	1.44 (1/fs)
HOMO	-4.94 (eV)
LUMO	-2.35 (eV)
Key	LJEXIGHVEZQWDQ
Weight	1011.29
SA Score	3.70
Color Est.	



Nicknamc	malika_June15_38-56
Splitting	0.101 (eV)
Strength	0.126
Absorption	2.61 (eV)
Rate	0.26 (1/fs)
HOMO	-4.81 (eV)
LUMO	-1.96 (eV)
Key	CTGCZGQYYXHILE
Weight	717.29
SA Score	2.59
Color Est.	



Nicknamc	malika_June15_39-57
Splitting	0.119 (eV)
Strength	0.228
Absorption	1.94 (eV)
Rate	0.12 (1/fs)
HOMO	-4.96 (eV)
LUMO	-2.81 (eV)
Key	YKYWBVATDHTPHS
Weight	714.28
SA Score	2.83
Color Est.	

FIGURE 57

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar4-5	0.161	0.348	2.64	0.07	-5.58	-2.69	OVQXOFBVMQQDRK	904.3	3.6
		oscar4-6	0.123	0.257	2.78	0.24	-4.92	-1.86	JLJQGQHCVXNCHE	957.4	3.6
		oscar4-7	0.142	0.239	2.84	0.11	-5.01	-1.91	GCRQIDXELSMBRT	929.3	3.3
		oscar4-10	0.152	0.147	2.86	0.05	-5.40	-2.24	QRHKKZYXEFRHIH	723.2	3.4
		oscar4-11	0.159	0.134	2.86	0.03	-4.95	-1.83	QYISDTKIZWLSAD	955.4	3.4
		oscar4-12	0.124	0.117	2.81	0.11	-5.00	-1.89	GWPTZBGJMLGERO	753.3	3.1
		oscar4-15	0.141	0.112	3.05	0.06	-5.16	-1.76	AMAUHYNTBIDALW	856.3	3.1

Table 5

FIGURE 58

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar4-16	0.138	0.112	2.75	0.06	-5.09	-2.03	NQAAVNJMKXCZAH	818.3	3.2
		oscar4-17	0.091	0.102	2.67	0.30	-4.54	-1.59	FLLUACRBLZWFQU	829.3	3.1
		oscar4-18	0.119	0.056	2.76	0.06	-5.01	-1.87	DQEQLXDYZAMQIO	862.3	2.9
		oscar4-19	0.103	0.055	2.83	0.12	-5.29	-2.19	VNCOABHYCXJYOB	1032.3	3.8
		oscar5-20	0.063	0.083	2.68	0.73	-5.33	-2.33	RHNBWQGVIRUTOR	794.3	2.7
		oscar6-21	0.142	0.098	2.84	0.05	-5.51	-2.35	LVDXGOXKTSSGQC	741.2	3.1
		oscar8-23	0.161	0.158	2.69	0.03	-5.38	-2.36	CTDLQVQASHTYEG	788.2	3.2

FIGURE 59

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar9-24	0.079	0.084	2.93	0.48	-5.46	-2.15	FKLBPQXHWGOSMX	796.3	3.0
		oscar10-25	0.082	0.055	2.81	0.26	-5.34	-2.15	JLELDKQARWLPIB	765.3	3.0
		oscar11-26	0.155	0.080	2.74	0.02	-5.28	-2.21	YCUKHVLEOSLWJF	732.2	3.4
		oscar12-27	0.097	0.094	2.79	0.25	-5.71	-2.40	KDAGQYKRGKUWSH	785.3	2.9
		oscar13-28	0.121	0.060	2.75	0.06	-4.71	-1.66	UKUAAOKXXJKJDY	587.2	2.5
		oscar15-30	0.122	0.169	2.65	0.15	-5.36	-2.38	UBCMMCIVRGOAAP	663.2	3.1
		oscar16-31	0.121	0.073	2.85	0.08	-5.53	-2.34	MVAGMKDMVOUPQS	693.1	3.3

FIGURE 60

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar17-32	0.170	0.071	3.00	0.01	-5.21	-1.96	AYSNDQVPDRIVKZ	719.2	3.2
		oscar19-34	0.101	0.059	2.83	0.13	-5.46	-2.13	GYFYCTDVYLJOHD	755.2	3.1
		oscar20-35	0.067	0.065	2.66	0.48	-4.98	-2.05	ZDSGGYMIEAGYLJ	755.3	3.0
		oscar21-36	0.159	0.192	2.75	0.05	-5.43	-2.32	KIYGZJGWFFEUCM	833.3	3.1
		oscar21-37	0.159	0.186	2.74	0.04	-5.46	-2.37	IVMVQYFGPYNUGE	879.3	3.2
		oscar22-38	0.167	0.231	3.05	0.05	-5.67	-2.29	IBNRKPXHRCMJRW	778.2	2.7
		oscar23-39	0.153	0.168	2.76	0.05	-4.97	-1.90	NHWVOKREZQWEKF	654.2	2.7

FIGURE 61

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar24-40	0.148	0.181	2.71	0.06	-5.58	-2.46	ROBJFXJOEHSEMX	690.1	3.1
		oscar24-42	0.135	0.168	2.79	0.10	-5.49	-2.31	QLVLLNJZXHEYCC	831.3	3.4
		oscar24-43	0.127	0.153	2.76	0.12	-5.79	-2.72	QUWUNIOXLSREHK	658.1	3.7
		oscar24-44	0.174	0.153	2.74	0.02	-5.05	-2.08	ZLFJXBLBYCGMRC	742.3	2.8
		oscar24-45	0.146	0.141	2.73	0.05	-5.10	-2.13	VTRKPAPVBJYARZ	738.3	3.3
		oscar24-46	0.161	0.131	2.89	0.03	-5.50	-2.23	HSJWVPVMKRNLQG	652.2	3.1
		oscar24-47	0.153	0.128	2.91	0.04	-5.66	-2.33	AOKDFCMNDUPRCF	892.1	3.5

FIGURE 62

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar24-48	0.159	0.124	2.82	0.03	-5.13	-1.99	ULKADLYDHXWPEQ	791.2	3.0
		oscar24-49	0.171	0.123	2.88	0.02	-5.52	-2.21	UXPHZMNNCVKJNK	604.2	2.8
		oscar24-50	0.138	0.119	2.77	0.06	-5.11	-2.04	WFQKJQPGRVOVIR	846.3	3.4
		oscar24-51	0.166	0.112	2.72	0.02	-5.04	-2.02	WOOVWEITLZYKQW	577.2	2.9
		oscar24-52	0.120	0.109	2.72	0.11	-4.83	-1.86	TXIRQNSGRSQTQW	699.2	2.9
		oscar24-54	0.171	0.104	2.79	0.02	-4.86	-1.76	KSDNBCJFCZPUCI	736.2	3.1
		oscar24-55	0.146	0.098	3.02	0.04	-5.48	-2.11	WJPMXDAPPRXZEQ	701.1	2.9

FIGURE 63

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar24-57	0.115	0.096	2.70	0.12	-5.44	-2.40	AAGDLUGMTFLIDD	590.2	3.0
		oscar24-61	0.157	0.091	2.65	0.02	-5.31	-2.35	WMBDKEBHVNQTFT	633.2	3.0
		oscar24-62	0.168	0.091	2.76	0.01	-4.87	-1.84	PCBKHHGOXYSKSU	641.3	2.9
		oscar24-65	0.128	0.084	2.80	0.07	-5.27	-2.24	LZYBGJYSRBDNNY	771.2	3.4
		oscar24-66	0.158	0.084	2.79	0.02	-5.03	-1.97	XMAVNOAGLQZJKX	758.2	3.1
		oscar24-67	0.134	0.082	2.87	0.06	-5.31	-2.19	LUTDEUKGVHVGAU	746.1	3.2
		oscar24-68	0.171	0.081	2.93	0.01	-5.34	-2.05	UCZJAZAELVDDNS	664.2	2.9

FIGURE 64

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar24-69	0.150	0.079	2.76	0.03	-4.93	-1.95	DPIBUHGSRGQBCL	811.3	3.3
		oscar24-70	0.164	0.079	2.76	0.02	-4.97	-1.96	CFWZIDTVSQVWHA	685.2	2.7
		oscar24-73	0.121	0.077	2.70	0.08	-5.18	-1.89	KEQMVFFVTFLIIZ	834.2	3.1
		oscar24-74	0.167	0.077	2.67	0.01	-5.47	-2.60	GRDVDFIBIPAWQL	726.2	3.3
		oscar24-77	0.142	0.070	2.72	0.03	-5.02	-2.07	RUCNMZBRUPXRPU	734.3	2.9
		oscar24-78	0.127	0.067	2.79	0.05	-5.56	-2.54	GJWPLLVLEKIESD	639.2	2.9
		oscar24-79	0.152	0.066	2.68	0.02	-4.96	-1.97	FFXDCRRWPIKQSH	642.2	2.8

FIGURE 65

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar24-81	0.169	0.064	2.72	0.01	-5.33	-2.23	VEFKFNINRKTFMC	697.2	3.0
		oscar24-82	0.148	0.062	2.75	0.02	-5.32	-2.22	TVBUFUCVTHYWQE	697.2	3.1
		oscar24-84	0.141	0.060	2.88	0.03	-5.16	-1.93	NZZYCMYWLHNPRT	680.2	3.0
		oscar24-85	0.133	0.060	2.76	0.04	-4.97	-2.00	HUENDXFMYWZKKW	781.3	3.1
		oscar24-86	0.163	0.059	2.94	0.01	-5.11	-1.90	JKNVSEGTUKDNCP	735.3	2.9
		oscar24-88	0.131	0.059	2.74	0.04	-4.79	-1.76	VCQBJHBATSQGMC	555.2	2.6
		oscar24-89	0.122	0.058	2.65	0.05	-4.92	-2.07	PZLPYRMJGQESMP	754.3	3.1

FIGURE 66

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar24-91	0.141	0.055	2.71	0.02	-4.94	-1.92	ABKZMNJPQUXOJR	685.2	2.9
		oscar24-94	0.127	0.054	2.73	0.04	-5.35	-2.23	XLTASWVPBGWOHN	660.2	3.0
		oscar24-95	0.170	0.053	2.94	0.01	-5.41	-2.15	ZYIDRDYBUMFBDT	781.2	3.2
		oscar24-96	0.156	0.052	3.04	0.02	-5.48	-1.86	RPTLFJQNHPZZEB	724.3	3.2
		oscar24-98	0.128	0.052	3.03	0.05	-5.47	-1.86	KKPDRGNSTXVZGH	708.3	3.2
		oscar24-100	0.172	0.051	2.82	0.01	-4.81	-1.77	AZNREJCVYIMBKH	760.3	3.0
		oscar24-103	0.123	0.050	2.79	0.05	-5.77	-2.66	WAMNAVJNSQJMRZ	852.2	3.0

FIGURE 67

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar25-105	0.123	0.071	2.82	0.07	-5.63	-2.43	ZFCARMGTPRWLCW	650.1	3.1
		oscar26-106	0.075	0.123	2.66	0.68	-6.18	-3.24	SZPTXKVEBYHAHN	894.2	3.4
		oscar28-108	0.140	0.161	3.04	0.09	-5.64	-2.20	VKQSCJVVOQSCJJ	717.2	2.9
		oscar29-109	0.159	0.173	2.77	0.04	-5.22	-2.07	MNIACRNZCKGZGH	922.3	3.6
		oscar30-111	0.133	0.073	2.73	0.04	-5.55	-2.55	HWYQKYKUZYKUGA	539.2	2.8
		oscar32-113	0.135	0.062	2.89	0.04	-5.33	-2.19	WOWBLWZRXJJJMM	718.2	3.3
		oscar33-114	0.139	0.149	3.06	0.09	-5.31	-1.90	WWOUZDMLFBXVQN	781.2	3.6

FIGURE 68

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar34-115	0.111	0.072	2.89	0.12	-5.53	-2.33	JUHKYTROZVDTEU	677.1	3.0
		oscar35-116	0.174	0.407	2.66	0.05	-5.59	-2.68	VGQLFPDWYOGLBI	920.2	3.6
		oscar35-117	0.161	0.076	2.81	0.02	-5.29	-2.14	XDOHNMWETVISFH	748.2	3.3
		oscar36-118	0.152	0.053	2.70	0.02	-5.86	-2.50	WDWSIDMEEUQHKU	816.2	2.9
		oscar37-119	0.157	0.121	3.17	0.04	-6.36	-2.92	LSHWWKJNHQPZKM	846.2	3.2
		oscar39-121	0.174	0.054	2.77	0.01	-5.07	-2.05	GBVAOWSQMXNMMC	679.3	3.1
		oscar40-122	0.138	0.052	2.72	0.03	-5.42	-2.38	ULIRBHJTYFLDPS	789.2	3.4

FIGURE 69

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar41-123	0.115	0.146	2.73	0.18	-5.10	-2.08	HHWUCNSNFAVETO	756.3	3.2
		oscar42-124	0.153	0.222	2.76	0.07	-4.93	-1.84	KQJPMJKMIGQLHO	850.4	3.3
		oscar43-125	0.153	0.067	2.80	0.02	-4.90	-1.87	OHFSABHEMLPINC	728.3	3.0
		oscar44-126	0.070	0.073	2.69	0.50	-5.73	-2.70	UYJNMZTXZCWANA	724.1	3.0
		oscar45-127	0.169	0.078	2.77	0.01	-5.45	-2.10	SYLKJBASCJQKSW	709.3	2.9
		oscar46-128	0.157	0.053	3.20	0.02	-4.99	-1.30	WHDUONAJIWKONZ	688.3	3.4
		oscar47-129	0.108	0.065	2.73	0.11	-5.59	-2.53	MAYQJXSWWXMIHF	637.1	2.9

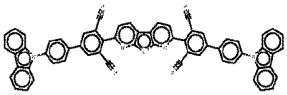
FIGURE 70

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar49-131	0.163	0.158	2.80	0.03	-5.44	-2.31	MMMBGODZJXAIBP	798.3	3.0
		oscar49-133	0.167	0.083	2.78	0.01	-5.47	-2.32	WCTPLTMHYGCGNX	721.3	2.9
		oscar50-134	0.119	0.053	2.79	0.06	-5.32	-2.18	YXACOVRWHKUYEE	915.3	3.3
		oscar51-135	0.075	0.063	2.69	0.35	-4.74	-1.74	SBDUVERFBWUSAC	601.2	2.8
		oscar54-138	0.111	0.099	2.66	0.14	-5.35	-2.37	FHLPYXCQFOTBKA	613.2	2.9
		oscar55-139	0.145	0.066	2.92	0.03	-5.21	-1.97	ICDBPFJXXFJKHL	810.2	3.2
		oscar56-140	0.174	0.078	2.79	0.01	-5.27	-2.28	DMLRTRGRUJEBNK	683.2	2.9

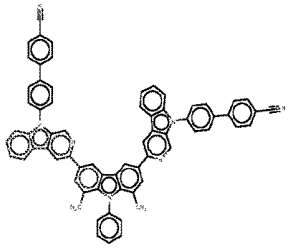
FIGURE 71

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		oscar57-141	0.077	0.061	2.72	0.33	-4.87	-1.91	ZMWOFDOGZLUWQC	754.3	2.9
		oscar58-142	0.143	0.051	2.96	0.03	-5.21	-2.02	DXYFVQBTANBEIO	613.2	2.7

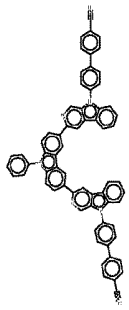
FIGURE 72



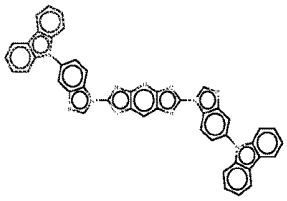
Nickname	oscar4-5
Splitting	0.161 (eV)
Strength	0.348
Absorption	2.64 (eV)
Rate	0.07 (1/us)
HOMO	-5.58 (eV)
LUMO	-2.69 (eV)
Key	OVQXOFBVMQQDRK
Weight	904.27
SA Score	3.69
Color Est.:	



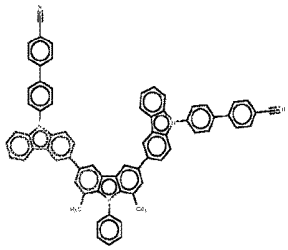
Nickname	oscar4-6
Splitting	0.123 (eV)
Strength	0.257
Absorption	2.78 (eV)
Rate	0.24 (1/us)
HOMO	-4.92 (eV)
LUMO	-1.88 (eV)
Key	JLJQGQHCVXNCHE
Weight	957.36
SA Score	3.61
Color Est.:	



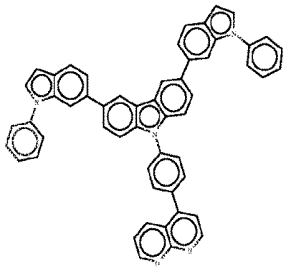
Nickname	oscar4-7
Splitting	0.142 (eV)
Strength	0.239
Absorption	2.84 (eV)
Rate	0.11 (1/us)
HOMO	-5.01 (eV)
LUMO	-1.91 (eV)
Key	GCRQIDXELSMBRT
Weight	929.33
SA Score	3.31
Color Est.:	



Nickname	oscar4-10
Splitting	0.152 (eV)
Strength	0.147
Absorption	2.86 (eV)
Rate	0.05 (1/us)
HOMO	-5.40 (eV)
LUMO	-2.24 (eV)
Key	QRHKKZYXEFRHH
Weight	723.21
SA Score	3.43
Color Est.:	



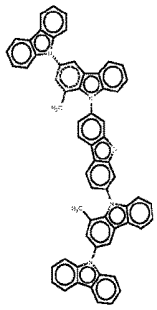
Nickname	oscar4-11
Splitting	0.159 (eV)
Strength	0.134
Absorption	2.86 (eV)
Rate	0.03 (1/us)
HOMO	-4.95 (eV)
LUMO	-1.83 (eV)
Key	QYISDTKIZWLSAD
Weight	955.37
SA Score	3.37
Color Est.:	



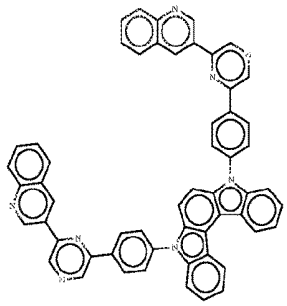
Nickname	oscar4-12
Splitting	0.124 (eV)
Strength	0.117
Absorption	2.81 (eV)
Rate	0.11 (1/us)
HOMO	-5.00 (eV)
LUMO	-1.89 (eV)
Key	GWPTZBGJMLGERO
Weight	753.29
SA Score	3.11
Color Est.:	

Table 6

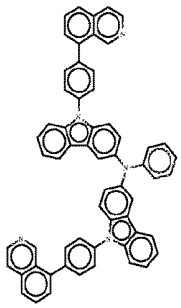
FIGURE 73



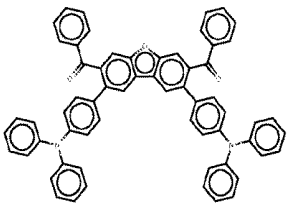
Nickname	oscar4-15
Splitting	0.141 (eV)
Strength	0.112
Absorption	3.05 (eV)
Rate	0.06 (1/us)
HOMO	-5.16 (eV)
LUMO	-1.76 (eV)
Key	AMAUHYNTBHDALW
Weight	856.32
SA Score	3.13
Color Est.:	



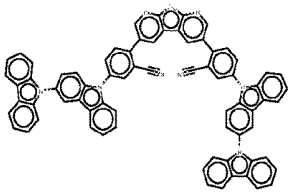
Nickname	oscar4-16
Splitting	0.138 (eV)
Strength	0.112
Absorption	2.75 (eV)
Rate	0.06 (1/us)
HOMO	-5.09 (eV)
LUMO	-2.03 (eV)
Key	NQAAVNJMKXCZAH
Weight	818.29
SA Score	3.20
Color Est.:	



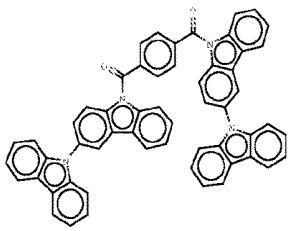
Nickname	oscar4-17
Splitting	0.091 (eV)
Strength	0.102
Absorption	2.67 (eV)
Rate	0.30 (1/us)
HOMO	-4.54 (eV)
LUMO	-1.59 (eV)
Key	FLLUACRBLZWFQU
Weight	829.32
SA Score	3.15
Color Est.:	



Nickname	oscar4-18
Splitting	0.119 (eV)
Strength	0.056
Absorption	2.76 (eV)
Rate	0.06 (1/us)
HOMO	-5.01 (eV)
LUMO	-1.87 (eV)
Key	DQEQLXDYZAMQIO
Weight	862.32
SA Score	2.93
Color Est.:	

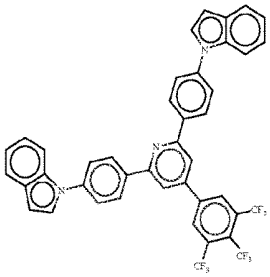


Nickname	oscar4-19
Splitting	0.403 (eV)
Strength	0.055
Absorption	2.83 (eV)
Rate	0.12 (1/us)
HOMO	-5.29 (eV)
LUMO	-2.19 (eV)
Key	VNOOABHYCXJYOB
Weight	1032.33
SA Score	3.79
Color Est.:	

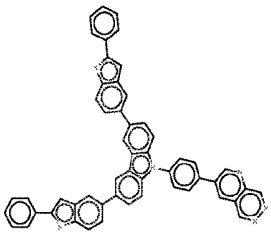


Nickname	oscar5-20
Splitting	0.063 (eV)
Strength	0.083
Absorption	2.68 (eV)
Rate	0.73 (1/us)
HOMO	-5.33 (eV)
LUMO	-2.33 (eV)
Key	RHNBWQGVIRUTOR
Weight	794.27
SA Score	2.72
Color Est.:	

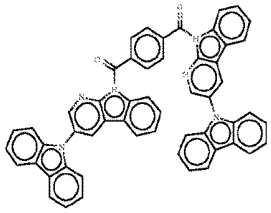
FIGURE 74



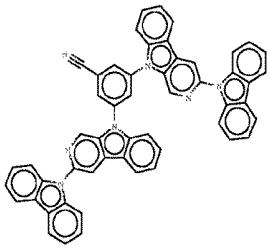
Nickname	oscar6-21
Splitting	0.142 (eV)
Strength	0.096
Absorption	2.84 (eV)
Rate	0.05 (1/us)
HOMO	-5.51 (eV)
LUMO	-2.35 (eV)
Key	LVDXGOXKTSSGQC
Weight	741.18
SA Score	3.05
Color Est.:	



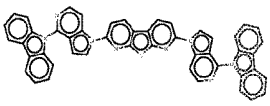
Nickname	oscar8-23
Splitting	0.161 (eV)
Strength	0.158
Absorption	2.69 (eV)
Rate	0.03 (1/us)
HOMO	-5.38 (eV)
LUMO	-2.36 (eV)
Key	CTDLQVQASHTYEO
Weight	788.21
SA Score	3.20
Color Est.:	



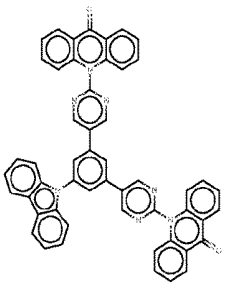
Nickname	oscar9-24
Splitting	0.079 (eV)
Strength	0.084
Absorption	2.93 (eV)
Rate	0.48 (1/us)
HOMO	-5.46 (eV)
LUMO	-2.15 (eV)
Key	FKLBPQXHWGOSMX
Weight	796.26
SA Score	3.01
Color Est.:	



Nickname	oscar10-25
Splitting	0.082 (eV)
Strength	0.055
Absorption	2.81 (eV)
Rate	0.26 (1/us)
HOMO	-5.34 (eV)
LUMO	-2.15 (eV)
Key	JLELDKQARWLPIB
Weight	765.26
SA Score	3.03
Color Est.:	

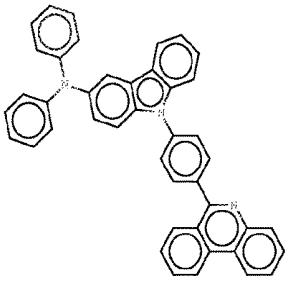


Nickname	oscar11-26
Splitting	0.155 (eV)
Strength	0.080
Absorption	2.74 (eV)
Rate	0.02 (1/us)
HOMO	-5.28 (eV)
LUMO	-2.21 (eV)
Key	YCUKHVLEOSLWJF
Weight	732.24
SA Score	3.35
Color Est.:	

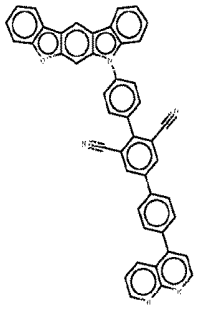


Nickname	oscar12-27
Splitting	0.097 (eV)
Strength	0.094
Absorption	2.79 (eV)
Rate	0.25 (1/us)
HOMO	-5.71 (eV)
LUMO	-2.49 (eV)
Key	KDAGQYKRGKUW8H
Weight	785.25
SA Score	2.94
Color Est.:	

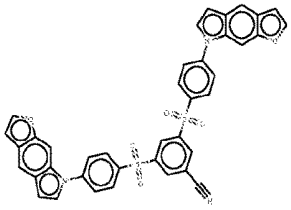
FIGURE 75



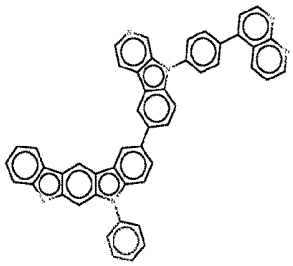
Nickname	oscar13-28
Splitting	0.121 (eV)
Strength	0.060
Absorption	2.75 (eV)
Rate	0.06 (1/ns)
HOMO	-4.71 (eV)
LUMO	-1.66 (eV)
Key	UKUAAOKXXJKJDY
Weight	587.24
SA Score	2.48
Color Est.:	



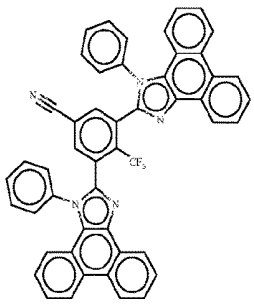
Nickname	oscar15-30
Splitting	0.122 (eV)
Strength	0.169
Absorption	2.65 (eV)
Rate	0.15 (1/ns)
HOMO	-5.36 (eV)
LUMO	-2.38 (eV)
Key	UBCMMCIVRGOAAP
Weight	663.21
SA Score	3.14
Color Est.:	



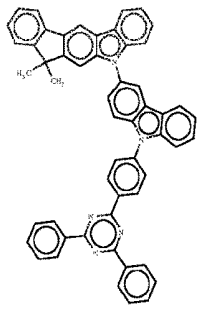
Nickname	oscar16-31
Splitting	0.121 (eV)
Strength	0.073
Absorption	2.85 (eV)
Rate	0.08 (1/ns)
HOMO	-5.53 (eV)
LUMO	-2.34 (eV)
Key	MVAGMKDMVOUPQS
Weight	693.10
SA Score	3.31
Color Est.:	



Nickname	oscar17-32
Splitting	0.170 (eV)
Strength	0.071
Absorption	3.00 (eV)
Rate	0.01 (1/ns)
HOMO	-5.21 (eV)
LUMO	-1.96 (eV)
Key	AYSNDQVPDRIVKZ
Weight	719.21
SA Score	3.17
Color Est.:	

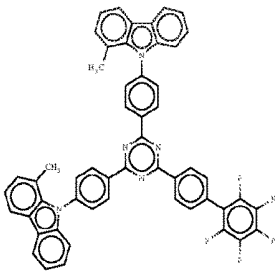


Nickname	oscar19-34
Splitting	0.101 (eV)
Strength	0.059
Absorption	2.83 (eV)
Rate	0.13 (1/ns)
HOMO	-5.46 (eV)
LUMO	-2.13 (eV)
Key	GYFYCTDVYLJOHD
Weight	755.23
SA Score	3.15
Color Est.:	

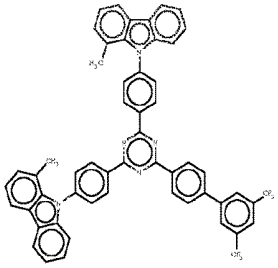


Nickname	oscar20-35
Splitting	0.067 (eV)
Strength	0.065
Absorption	2.66 (eV)
Rate	0.48 (1/ns)
HOMO	-4.98 (eV)
LUMO	-2.05 (eV)
Key	ZDSGGYMEAGYLJ
Weight	755.30
SA Score	2.98
Color Est.:	

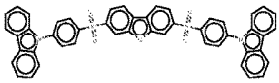
FIGURE 76



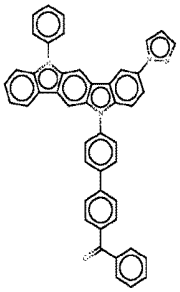
Nickname	oscar21-36
Splitting	0.159 (eV)
Strength	0.192
Absorption	2.75 (eV)
Rate	0.05 (1/us)
HOMO	-5.43 (eV)
LUMO	-2.32 (eV)
Key	KJYGZJGWFFEUCM
Weight	833.26
SA Score	3.12
Color Est.:	



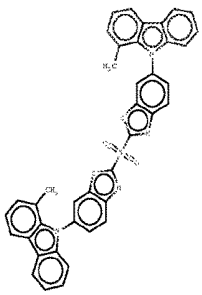
Nickname	oscar21-37
Splitting	0.159 (eV)
Strength	0.186
Absorption	2.74 (eV)
Rate	0.04 (1/us)
HOMO	-5.46 (eV)
LUMO	-2.37 (eV)
Key	IVMVQYFGPYNUGE
Weight	879.28
SA Score	3.19
Color Est.:	



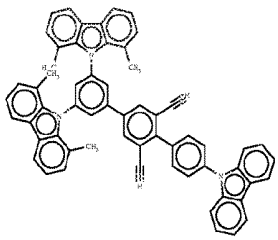
Nickname	oscar22-38
Splitting	0.167 (eV)
Strength	0.231
Absorption	3.05 (eV)
Rate	0.05 (1/us)
HOMO	-5.67 (eV)
LUMO	-2.29 (eV)
Key	IBNRKPXHRCMJRW
Weight	778.16
SA Score	2.67
Color Est.:	



Nickname	oscar23-39
Splitting	0.153 (eV)
Strength	0.168
Absorption	2.76 (eV)
Rate	0.05 (1/us)
HOMO	-4.97 (eV)
LUMO	-1.90 (eV)
Key	NHWVOKREZQWEKF
Weight	654.24
SA Score	2.75
Color Est.:	

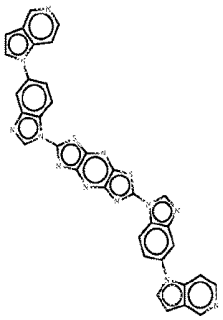


Nickname	oscar24-40
Splitting	0.148 (eV)
Strength	0.181
Absorption	2.71 (eV)
Rate	0.06 (1/us)
HOMO	-5.58 (eV)
LUMO	-2.46 (eV)
Key	ROBJFXJOEHSEMX
Weight	690.12
SA Score	3.11
Color Est.:	

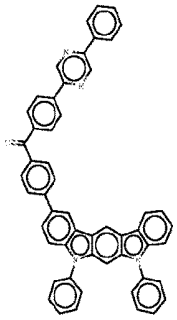


Nickname	oscar24-42
Splitting	0.135 (eV)
Strength	0.168
Absorption	2.79 (eV)
Rate	0.10 (1/us)
HOMO	-5.49 (eV)
LUMO	-2.31 (eV)
Key	QLVLLNJZXHEYCC
Weight	831.34
SA Score	3.40
Color Est.:	

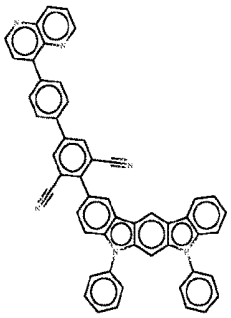
FIGURE 77



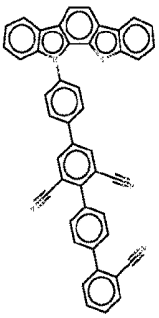
Nickname	oscar24-43
Splitting	0.127 (eV)
Strength	0.153
Absorption	2.76 (eV)
Rate	0.12 (1/us)
HOMO	-5.79 (eV)
LUMO	-2.72 (eV)
Key	QUWUNHOXLSREHK
Weight	658.12
SA Score	3.70
Color Est.:	



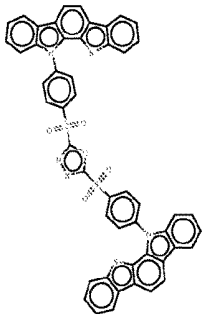
Nickname	oscar24-44
Splitting	0.174 (eV)
Strength	0.153
Absorption	2.74 (eV)
Rate	0.02 (1/us)
HOMO	-5.05 (eV)
LUMO	-2.08 (eV)
Key	ZLFIXBLBYCGMRC
Weight	742.27
SA Score	2.82
Color Est.:	



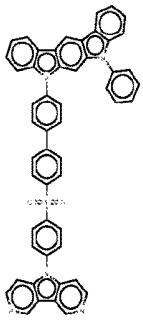
Nickname	oscar24-45
Splitting	0.146 (eV)
Strength	0.141
Absorption	2.73 (eV)
Rate	0.05 (1/us)
HOMO	-5.10 (eV)
LUMO	-2.13 (eV)
Key	VTRKPAPVBJYARZ
Weight	738.25
SA Score	3.26
Color Est.:	



Nickname	oscar24-46
Splitting	0.161 (eV)
Strength	0.131
Absorption	2.89 (eV)
Rate	0.03 (1/us)
HOMO	-5.50 (eV)
LUMO	-2.23 (eV)
Key	HSJWVPVMKRNLQG
Weight	652.17
SA Score	3.05
Color Est.:	

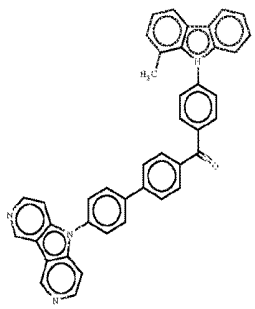


Nickname	oscar24-47
Splitting	0.153 (eV)
Strength	0.128
Absorption	2.91 (eV)
Rate	0.04 (1/us)
HOMO	-5.66 (eV)
LUMO	-2.33 (eV)
Key	AOKDFCMNDUPRCF
Weight	892.09
SA Score	3.46
Color Est.:	

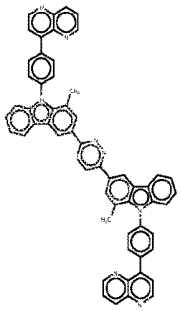


Nickname	oscar24-48
Splitting	0.159 (eV)
Strength	0.124
Absorption	2.82 (eV)
Rate	0.03 (1/us)
HOMO	-5.13 (eV)
LUMO	-1.99 (eV)
Key	ULKADLYDHXWPEQ
Weight	791.24
SA Score	2.99
Color Est.:	

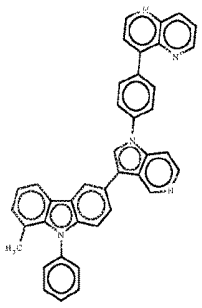
FIGURE 78



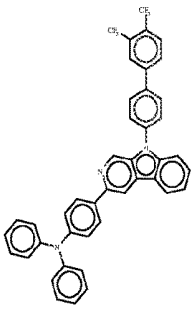
Nickname	oscar24-49
Splitting	0.171 (eV)
Strength	0.123
Absorption	2.88 (eV)
Rate	0.02 (1/ns)
HOMO	-5.52 (eV)
LUMO	-2.21 (eV)
Key	UXPHZMNNCVEJNK
Weight	604.23
SA Score	2.75
Color Est.:	



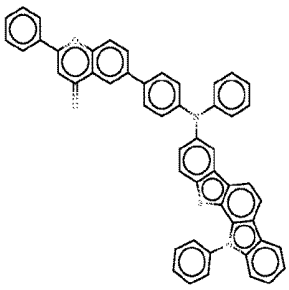
Nickname	oscar24-50
Splitting	0.138 (eV)
Strength	0.119
Absorption	2.77 (eV)
Rate	0.06 (1/ns)
HOMO	-5.31 (eV)
LUMO	-2.04 (eV)
Key	WFQKJQPGRVOVIR
Weight	846.32
SA Score	3.44
Color Est.:	



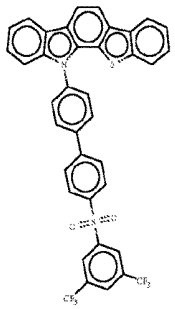
Nickname	oscar24-51
Splitting	0.166 (eV)
Strength	0.112
Absorption	2.72 (eV)
Rate	0.02 (1/ns)
HOMO	-5.04 (eV)
LUMO	-2.02 (eV)
Key	WOOVWEITLZYKQW
Weight	577.23
SA Score	2.86
Color Est.:	



Nickname	oscar24-52
Splitting	0.120 (eV)
Strength	0.109
Absorption	2.72 (eV)
Rate	0.11 (1/ns)
HOMO	-4.83 (eV)
LUMO	-1.86 (eV)
Key	TXIRQNSGRSQTQW
Weight	699.21
SA Score	2.91
Color Est.:	

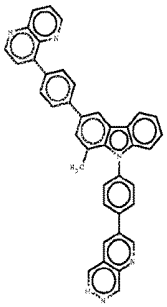


Nickname	oscar24-54
Splitting	0.171 (eV)
Strength	0.104
Absorption	2.79 (eV)
Rate	0.02 (1/ns)
HOMO	-4.86 (eV)
LUMO	-1.76 (eV)
Key	KSDNBCJFCZPUCI
Weight	736.22
SA Score	3.07
Color Est.:	

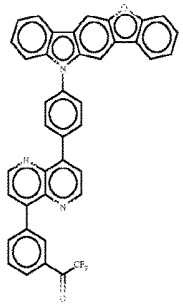


Nickname	oscar24-55
Splitting	0.146 (eV)
Strength	0.098
Absorption	3.02 (eV)
Rate	0.04 (1/ns)
HOMO	-5.48 (eV)
LUMO	-2.11 (eV)
Key	WJPMXDAPPRXZEQ
Weight	701.09
SA Score	2.91
Color Est.:	

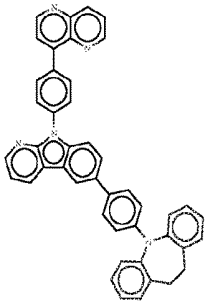
FIGURE 79



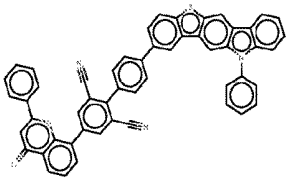
Nickname	oscar24-57
Splitting	0.115 (eV)
Strength	0.096
Absorption	2.70 (eV)
Rate	0.12 (1/us)
HOMO	-5.44 (eV)
LUMO	-2.40 (eV)
Key	AAGDLUGMTFLIDD
Weight	590.22
SA Score	2.96
Color Est.:	



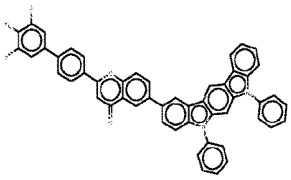
Nickname	oscar24-61
Splitting	0.157 (eV)
Strength	0.091
Absorption	2.65 (eV)
Rate	0.02 (1/us)
HOMO	-5.31 (eV)
LUMO	-2.35 (eV)
Key	WMBDKEBHVNQTFT
Weight	633.17
SA Score	2.98
Color Est.:	



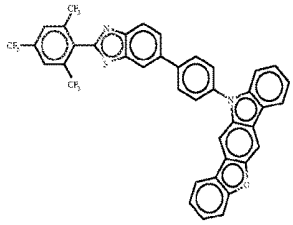
Nickname	oscar24-62
Splitting	0.168 (eV)
Strength	0.091
Absorption	2.76 (eV)
Rate	0.04 (1/us)
HOMO	-4.87 (eV)
LUMO	-1.84 (eV)
Key	PCBKHHGOXYSKSU
Weight	641.26
SA Score	2.87
Color Est.:	



Nickname	oscar24-65
Splitting	0.128 (eV)
Strength	0.084
Absorption	2.80 (eV)
Rate	0.07 (1/us)
HOMO	-5.27 (eV)
LUMO	-2.24 (eV)
Key	LZYBGJYSRBDNNY
Weight	771.20
SA Score	3.35
Color Est.:	

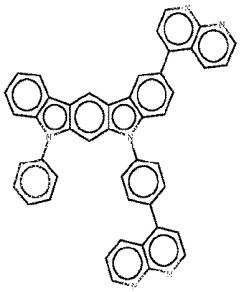


Nickname	oscar24-66
Splitting	0.158 (eV)
Strength	0.084
Absorption	2.79 (eV)
Rate	0.02 (1/us)
HOMO	-5.03 (eV)
LUMO	-1.97 (eV)
Key	XMAVNOAGLQZJKX
Weight	758.22
SA Score	3.05
Color Est.:	

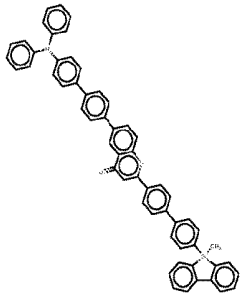


Nickname	oscar24-67
Splitting	0.134 (eV)
Strength	0.082
Absorption	2.87 (eV)
Rate	0.06 (1/us)
HOMO	-5.31 (eV)
LUMO	-2.19 (eV)
Key	LUTDEUKGVHVGAU
Weight	746.11
SA Score	3.19
Color Est.:	

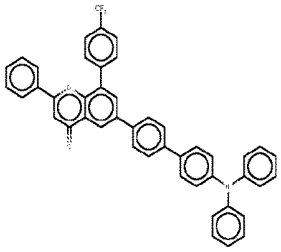
FIGURE 80



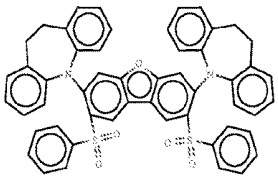
Nickname	oscar24-68
Splitting	0.171 (eV)
Strength	0.081
Absorption	2.93 (eV)
Rate	0.01 (1/ns)
HOMO	-5.34 (eV)
LUMO	-2.05 (eV)
Key	UCZJAZAELVDDNS
Weight	664.24
SA Score	2.92
Color Est.:	



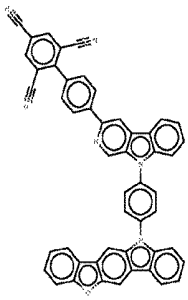
Nickname	oscar24-69
Splitting	0.150 (eV)
Strength	0.079
Absorption	2.76 (eV)
Rate	0.03 (1/ns)
HOMO	-4.93 (eV)
LUMO	-1.95 (eV)
Key	DPIBUHGSRGQBCL
Weight	811.29
SA Score	3.27
Color Est.:	



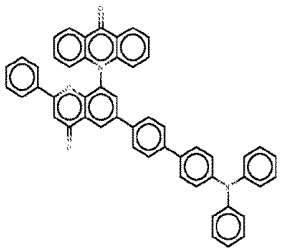
Nickname	oscar24-70
Splitting	0.164 (eV)
Strength	0.079
Absorption	2.76 (eV)
Rate	0.02 (1/ns)
HOMO	-4.97 (eV)
LUMO	-1.96 (eV)
Key	CFWZIDTVSQVWHA
Weight	685.22
SA Score	2.72
Color Est.:	



Nickname	oscar24-73
Splitting	0.121 (eV)
Strength	0.077
Absorption	2.70 (eV)
Rate	0.08 (1/ns)
HOMO	-5.18 (eV)
LUMO	-1.89 (eV)
Key	KEQMVFFVTFLHZ
Weight	834.22
SA Score	3.12
Color Est.:	

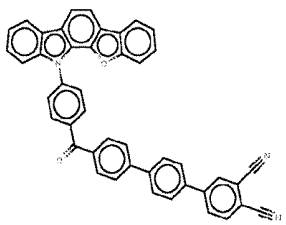


Nickname	oscar24-74
Splitting	0.167 (eV)
Strength	0.077
Absorption	2.67 (eV)
Rate	0.01 (1/ns)
HOMO	-5.47 (eV)
LUMO	-2.60 (eV)
Key	GRDVDFIBIPAWQL
Weight	726.22
SA Score	3.35
Color Est.:	

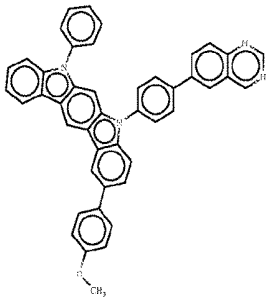


Nickname	oscar24-77
Splitting	0.142 (eV)
Strength	0.070
Absorption	2.72 (eV)
Rate	0.03 (1/ns)
HOMO	-5.02 (eV)
LUMO	-2.07 (eV)
Key	RUCNMZBRUPXRPU
Weight	734.26
SA Score	2.88
Color Est.:	

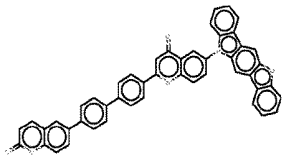
FIGURE 81



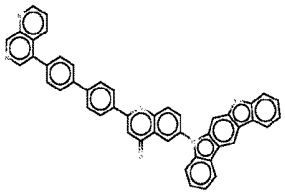
Nickname	oscar24-78
Splitting	0.127 (eV)
Strength	0.067
Absorption	2.79 (eV)
Rate	0.05 (1/us)
HOMO	-5.56 (eV)
LUMO	-2.54 (eV)
Key	GJWPLLVLEKJESD
Weight	639.19
SA Score	2.86
Color Est.:	



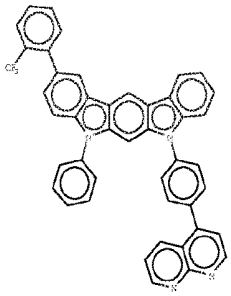
Nickname	oscar24-79
Splitting	0.152 (eV)
Strength	0.066
Absorption	2.68 (eV)
Rate	0.02 (1/us)
HOMO	-4.96 (eV)
LUMO	-1.97 (eV)
Key	FFXDCRRWPIKQSH
Weight	642.24
SA Score	2.79
Color Est.:	



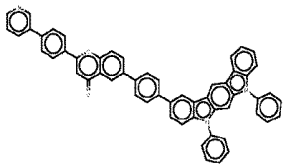
Nickname	oscar24-81
Splitting	0.169 (eV)
Strength	0.064
Absorption	2.72 (eV)
Rate	0.01 (1/us)
HOMO	-5.33 (eV)
LUMO	-2.23 (eV)
Key	VEFKFNINRKTFMC
Weight	697.19
SA Score	3.03
Color Est.:	



Nickname	oscar24-82
Splitting	0.148 (eV)
Strength	0.062
Absorption	2.75 (eV)
Rate	0.02 (1/us)
HOMO	-5.32 (eV)
LUMO	-2.22 (eV)
Key	TVBUFUCVTHYWQE
Weight	697.18
SA Score	3.07
Color Est.:	

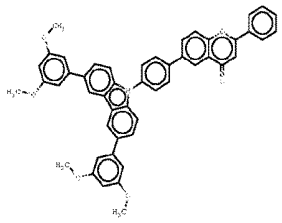


Nickname	oscar24-84
Splitting	0.141 (eV)
Strength	0.060
Absorption	2.88 (eV)
Rate	0.03 (1/us)
HOMO	-5.16 (eV)
LUMO	-1.93 (eV)
Key	NZZYCMYWLHNPRT
Weight	680.22
SA Score	2.97
Color Est.:	

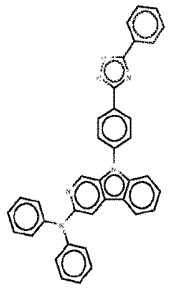


Nickname	oscar24-85
Splitting	0.133 (eV)
Strength	0.060
Absorption	2.76 (eV)
Rate	0.04 (1/us)
HOMO	-4.97 (eV)
LUMO	-2.00 (eV)
Key	HUENDXFMYWZKKW
Weight	781.27
SA Score	3.06
Color Est.:	

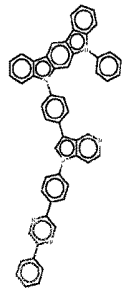
FIGURE 82



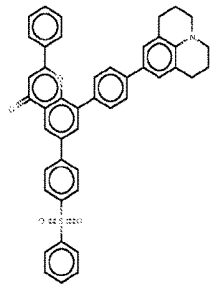
Nickname	oscar24-86
Splitting	0.163 (eV)
Strength	0.059
Absorption	2.94 (eV)
Rate	0.01 (1/us)
HOMO	-5.11 (eV)
LUMO	-1.90 (eV)
Key	JKNVSEGTUKDNCP
Weight	735.26
SA Score	2.89
Color Est.:	



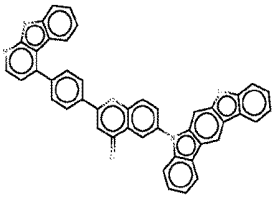
Nickname	oscar24-88
Splitting	0.131 (eV)
Strength	0.059
Absorption	2.74 (eV)
Rate	0.04 (1/us)
HOMO	-4.79 (eV)
LUMO	-1.76 (eV)
Key	VOGBJHBATSQGMC
Weight	555.21
SA Score	2.59
Color Est.:	



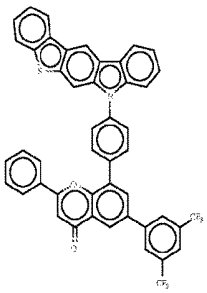
Nickname	oscar24-89
Splitting	0.122 (eV)
Strength	0.058
Absorption	2.65 (eV)
Rate	0.05 (1/us)
HOMO	-4.92 (eV)
LUMO	-2.07 (eV)
Key	PZLPYRMJGQESMP
Weight	754.28
SA Score	3.09
Color Est.:	



Nickname	oscar24-91
Splitting	0.141 (eV)
Strength	0.055
Absorption	2.71 (eV)
Rate	0.02 (1/us)
HOMO	-4.94 (eV)
LUMO	-1.92 (eV)
Key	ABKZMNJPQUNOJR
Weight	685.23
SA Score	2.92
Color Est.:	

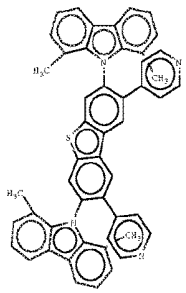


Nickname	oscar24-94
Splitting	0.127 (eV)
Strength	0.054
Absorption	2.73 (eV)
Rate	0.04 (1/us)
HOMO	-5.35 (eV)
LUMO	-2.23 (eV)
Key	XLTASWVPBGWOHN
Weight	660.15
SA Score	3.03
Color Est.:	

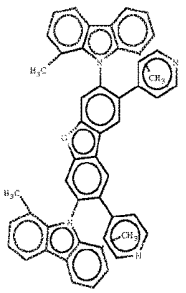


Nickname	oscar24-95
Splitting	0.170 (eV)
Strength	0.053
Absorption	2.94 (eV)
Rate	0.01 (1/us)
HOMO	-5.41 (eV)
LUMO	-2.15 (eV)
Key	ZYIDRDYBUMFBDT
Weight	781.15
SA Score	3.24
Color Est.:	

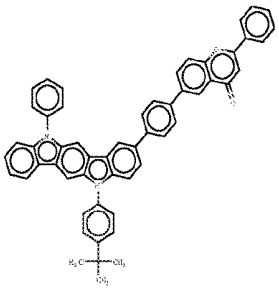
FIGURE 83



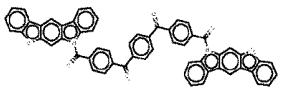
Nickname	oscar24-96
Splitting	0.156 (eV)
Strength	0.052
Absorption	3.04 (eV)
Rate	0.02 (1/us)
HOMO	-5.48 (eV)
LUMO	-1.86 (eV)
Key	RPTLFJQMHPZZEB
Weight	724.27
SA Score	3.24
Color Est.:	



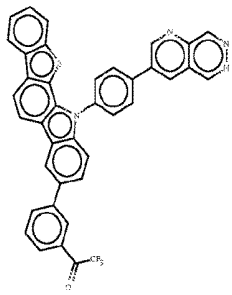
Nickname	oscar24-98
Splitting	0.128 (eV)
Strength	0.052
Absorption	3.03 (eV)
Rate	0.05 (1/us)
HOMO	-5.47 (eV)
LUMO	-1.86 (eV)
Key	KKPDRONSTXVZGH
Weight	708.29
SA Score	3.19
Color Est.:	



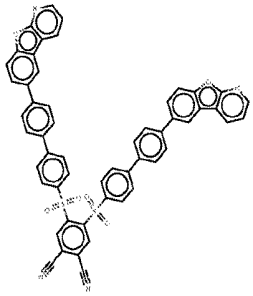
Nickname	oscar24-109
Splitting	0.172 (eV)
Strength	0.051
Absorption	2.82 (eV)
Rate	0.01 (1/us)
HOMO	-4.81 (eV)
LUMO	-1.77 (eV)
Key	AZNREJCVYIMBKH
Weight	760.31
SA Score	3.01
Color Est.	



Nickname	oscar24-103
Splitting	0.123 (eV)
Strength	0.050
Absorption	2.79 (eV)
Rate	0.05 (1/us)
HOMO	-5.77 (eV)
LUMO	-2.66 (eV)
Key	WAMNAVJNSQJMRZ
Weight	852.23
SA Score	3.05
Color Est.:	

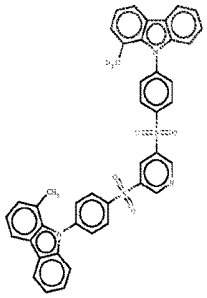


Nickname	oscar25-105
Splitting	0.123 (eV)
Strength	0.071
Absorption	2.82 (eV)
Rate	0.07 (1/us)
HOMO	-5.63 (eV)
LUMO	-2.43 (eV)
Key	ZPCARMGTPRWLCW
Weight	650.14
SA Score	3.14
Color Est.:	

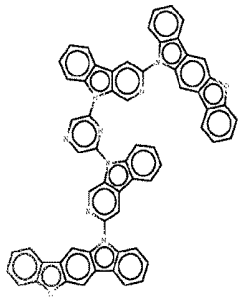


Nickname	oscar26-106
Splitting	0.075 (eV)
Strength	0.123
Absorption	2.66 (eV)
Rate	0.68 (1/us)
HOMO	-6.18 (eV)
LUMO	-3.24 (eV)
Key	SZPTXKVEBYHAHN
Weight	894.16
SA Score	3.39
Color Est.	

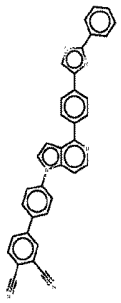
FIGURE 84



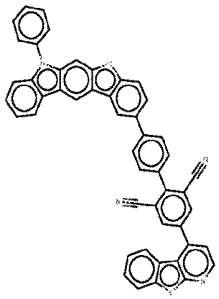
Nickname	oscar28-108
Splitting	0.140 (eV)
Strength	0.161
Absorption	3.04 (eV)
Rate	0.09 (1/us)
HOMO	-5.64 (eV)
LUMO	-2.20 (eV)
Key	VKQSCJVVOQSCIJ
Weight	717.18
SA Score	2.87
Color Est.:	



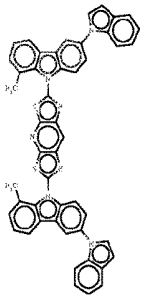
Nickname	oscar29-109
Splitting	0.139 (eV)
Strength	0.173
Absorption	2.77 (eV)
Rate	0.04 (1/us)
HOMO	-5.22 (eV)
LUMO	-2.07 (eV)
Key	MNIACRNZCKGZGH
Weight	922.28
SA Score	3.64
Color Est.:	



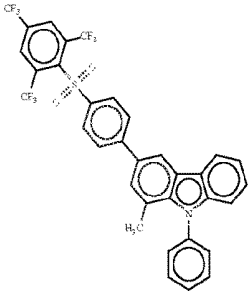
Nickname	oscar30-111
Splitting	0.133 (eV)
Strength	0.073
Absorption	2.73 (eV)
Rate	0.04 (1/us)
HOMO	-5.55 (eV)
LUMO	-2.55 (eV)
Key	HWYQKYKUZYKUGA
Weight	539.17
SA Score	2.80
Color Est.:	



Nickname	oscar32-113
Splitting	0.135 (eV)
Strength	0.062
Absorption	2.89 (eV)
Rate	0.04 (1/us)
HOMO	-5.33 (eV)
LUMO	-2.19 (eV)
Key	WGWBLWZRXJJMM
Weight	718.18
SA Score	3.28
Color Est.:	

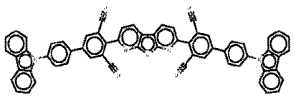


Nickname	oscar33-114
Splitting	0.139 (eV)
Strength	0.149
Absorption	3.06 (eV)
Rate	0.09 (1/us)
HOMO	-5.31 (eV)
LUMO	-1.90 (eV)
Key	WWOUZDMLFBXVQN
Weight	781.21
SA Score	3.58
Color Est.:	

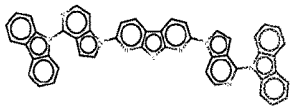


Nickname	oscar34-115
Splitting	0.111 (eV)
Strength	0.072
Absorption	2.89 (eV)
Rate	0.12 (1/us)
HOMO	-5.53 (eV)
LUMO	-2.33 (eV)
Key	JUHKYTROZVDTEU
Weight	677.11
SA Score	2.97
Color Est.:	

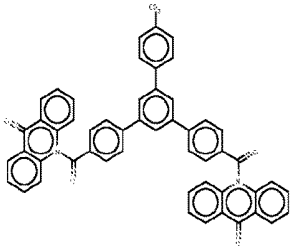
FIGURE 85



Nickname	oscar35-116
Splitting	0.174 (eV)
Strength	0.407
Absorption	2.66 (eV)
Rate	0.05 (1/ns)
HOMO	-5.59 (eV)
LUMO	-2.68 (eV)
Key	VGQLFFDWYOGLBI
Weight	920.25
SA Score	3.57
Color Est.:	

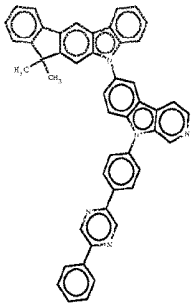


Nickname	oscar35-117
Splitting	0.161 (eV)
Strength	0.076
Absorption	2.81 (eV)
Rate	0.02 (1/ns)
HOMO	-5.29 (eV)
LUMO	-2.14 (eV)
Key	XDOHNMWETVISFH
Weight	748.22
SA Score	3.29
Color Est.:	

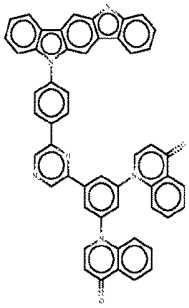


Nickname	oscar36-118
Splitting	0.152 (eV)
Strength	0.053
Absorption	2.70 (eV)
Rate	0.02 (1/ns)
HOMO	-5.86 (eV)
LUMO	-2.50 (eV)
Key	WDWSIDMEEUQHKU
Weight	816.22
SA Score	2.85
Color Est.:	

Nickname	oscar37-119
Splitting	0.157 (eV)
Strength	0.121
Absorption	3.17 (eV)
Rate	0.04 (1/ns)
HOMO	-6.36 (eV)
LUMO	-2.92 (eV)
Key	LSHWVKJNHQPZKM
Weight	846.18
SA Score	3.23
Color Est.:	

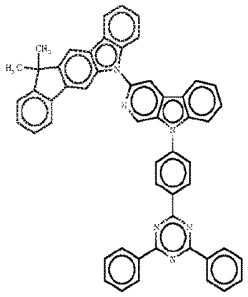


Nickname	oscar39-121
Splitting	0.174 (eV)
Strength	0.054
Absorption	2.77 (eV)
Rate	0.01 (1/ns)
HOMO	-5.07 (eV)
LUMO	-2.05 (eV)
Key	GBVAOWSQMXNMMC
Weight	679.27
SA Score	3.09
Color Est.:	

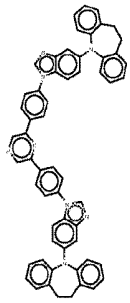


Nickname	oscar40-122
Splitting	0.138 (eV)
Strength	0.052
Absorption	2.72 (eV)
Rate	0.03 (1/ns)
HOMO	-5.42 (eV)
LUMO	-2.38 (eV)
Key	ULIRBHJTYFLDPS
Weight	789.22
SA Score	3.44
Color Est.:	

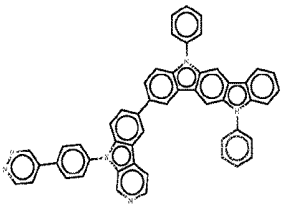
FIGURE 86



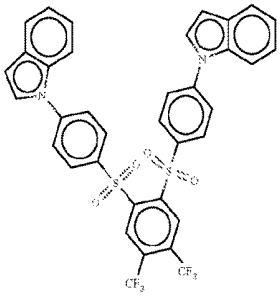
Nickname	oscar41-123
Splitting	0.115 (eV)
Strength	0.146
Absorption	2.73 (eV)
Rate	0.18 (1/us)
HOMO	-5.10 (eV)
LUMO	-2.08 (eV)
Key	HHWUCNSNFAVETO
Weight	756.30
SA Score	3.16
Color Est.:	



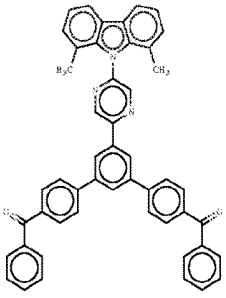
Nickname	oscar42-124
Splitting	0.153 (eV)
Strength	0.222
Absorption	2.76 (eV)
Rate	0.07 (1/us)
HOMO	-4.93 (eV)
LUMO	-1.84 (eV)
Key	KQJPMJKMHGQLHO
Weight	850.35
SA Score	3.29
Color Est.:	



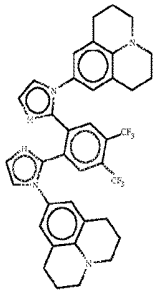
Nickname	oscar43-125
Splitting	0.153 (eV)
Strength	0.067
Absorption	2.80 (eV)
Rate	0.02 (1/us)
HOMO	-4.90 (eV)
LUMO	-1.87 (eV)
Key	OBFSABHEMLPINC
Weight	728.27
SA Score	3.01
Color Est.:	



Nickname	oscar44-126
Splitting	0.070 (eV)
Strength	0.073
Absorption	2.69 (eV)
Rate	0.50 (1/us)
HOMO	-5.73 (eV)
LUMO	-2.70 (eV)
Key	UYJNMZTXZCWANA
Weight	724.09
SA Score	2.96
Color Est.:	

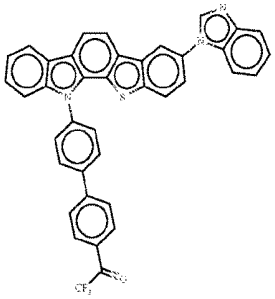


Nickname	oscar45-127
Splitting	0.169 (eV)
Strength	0.078
Absorption	2.77 (eV)
Rate	0.01 (1/us)
HOMO	-5.45 (eV)
LUMO	-2.10 (eV)
Key	SYLKJBASCJQKSW
Weight	709.27
SA Score	2.90
Color Est.:	

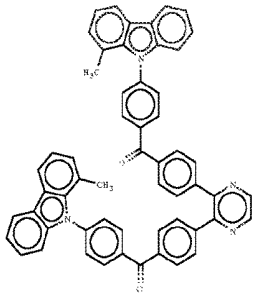


Nickname	oscar46-128
Splitting	0.157 (eV)
Strength	0.053
Absorption	3.20 (eV)
Rate	0.02 (1/us)
HOMO	-4.99 (eV)
LUMO	-1.30 (eV)
Key	WHDUONAJIWKONZ
Weight	688.27
SA Score	3.44
Color Est.:	

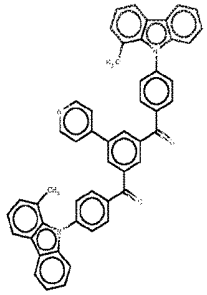
FIGURE 87



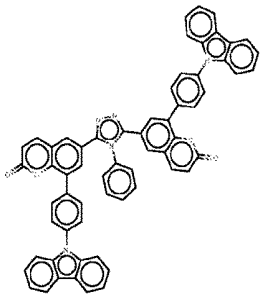
Nickname	oscar47-129
Splitting	0.108 (eV)
Strength	0.065
Absorption	2.73 (eV)
Rate	0.11 (1/us)
HOMO	-5.59 (eV)
LUMO	-2.52 (eV)
Key	MAYQJXSWWXMIHF
Weight	637.14
SA Score	2.91
Color Est.:	



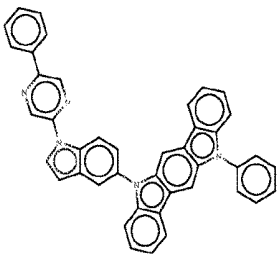
Nickname	oscar49-131
Splitting	0.163 (eV)
Strength	0.158
Absorption	2.80 (eV)
Rate	0.03 (1/us)
HOMO	-5.44 (eV)
LUMO	-2.31 (eV)
Key	MMMBGODZJXAIBP
Weight	798.30
SA Score	2.96
Color Est.:	



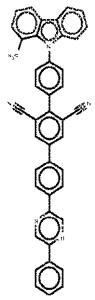
Nickname	oscar49-133
Splitting	0.167 (eV)
Strength	0.083
Absorption	2.78 (eV)
Rate	0.01 (1/us)
HOMO	-5.47 (eV)
LUMO	-2.32 (eV)
Key	WCTPLTMHYGCGNX
Weight	721.27
SA Score	2.91
Color Est.:	



Nickname	oscar50-134
Splitting	0.119 (eV)
Strength	0.053
Absorption	2.79 (eV)
Rate	0.06 (1/us)
HOMO	-5.32 (eV)
LUMO	-2.18 (eV)
Key	YXACOVRWHKUYEE
Weight	915.28
SA Score	3.34
Color Est.:	

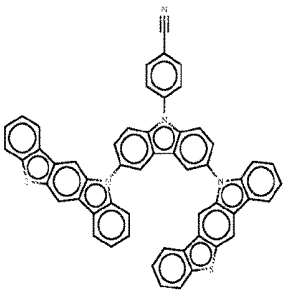


Nickname	oscar51-135
Splitting	0.075 (eV)
Strength	0.063
Absorption	2.69 (eV)
Rate	0.35 (1/us)
HOMO	-4.74 (eV)
LUMO	-1.74 (eV)
Key	SBDUVERFBWUSAC
Weight	601.23
SA Score	2.83
Color Est.:	

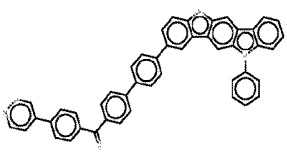


Nickname	oscar54-138
Splitting	0.111 (eV)
Strength	0.099
Absorption	2.66 (eV)
Rate	0.14 (1/us)
HOMO	-5.35 (eV)
LUMO	-2.37 (eV)
Key	FHLFYXCQFOTBKA
Weight	613.23
SA Score	2.91
Color Est.:	

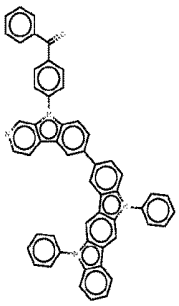
FIGURE 88



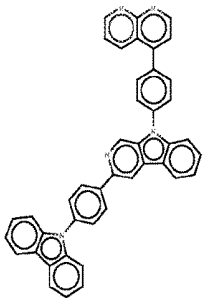
Nickname	oscar55-139
Splitting	0.145 (eV)
Strength	0.066
Absorption	2.92 (eV)
Rate	0.03 (1/us)
HOMO	-5.21 (eV)
LUMO	-1.97 (eV)
Key	ICDBPFJXXFJKHL
Weight	810.19
SA Score	3.15
Color Est.:	



Nickname	oscar56-140
Splitting	0.174 (eV)
Strength	0.078
Absorption	2.79 (eV)
Rate	0.04 (1/us)
HOMO	-5.27 (eV)
LUMO	-2.28 (eV)
Key	DMLRTRGRUJEBNK
Weight	683.20
SA Score	2.91
Color Est.:	



Nickname	oscar57-141
Splitting	0.077 (eV)
Strength	0.061
Absorption	2.72 (eV)
Rate	0.33 (1/us)
HOMO	-4.87 (eV)
LUMO	-1.91 (eV)
Key	ZMWOFDOGZLUWQC
Weight	754.27
SA Score	2.91
Color Est.:	



Nickname	oscar58-142
Splitting	0.143 (eV)
Strength	0.051
Absorption	2.96 (eV)
Rate	0.03 (1/us)
HOMO	-5.21 (eV)
LUMO	-2.02 (eV)
Key	DXYFVQBTANBEHO
Weight	613.23
SA Score	2.69
Color Est.:	

FIGURE 89

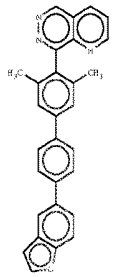
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		quebec-1	0.141	0.035	2.90	0.02	-5.56	-2.21	NAOLMGTWCVCQLN	427.2	2.6
		quebec-2	0.166	0.012	2.84	0.00	-5.66	-2.42	HOHSBCOUWGWHSN	522.2	3.0
		quebec-3	0.116	0.036	2.79	0.05	-5.37	-2.17	JYQURBPZOYNSHP	522.2	3.1
		quebec-5	0.135	0.075	2.81	0.05	-5.40	-2.21	FEAWYSMGXAAHEH	634.2	3.3
		quebec-6	0.169	0.098	2.85	0.02	-5.44	-2.21	SJYRYFHHVZQOKN	650.2	3.3
		quebec-7	0.155	0.047	2.94	0.01	-5.57	-2.19	YYDAGVMGKQCLNP	634.2	3.2
		quebec-8	0.085	0.027	2.83	0.12	-5.42	-2.23	LVWRADBSUWLHOE	650.2	3.3

Table 7

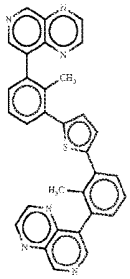
FIGURE 90

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		quebec-9	0.120	0.016	2.81	0.02	-6.22	-3.02	COWVQULBZVWOPZ	790.2	3.3
		quebec-10	0.090	0.010	2.69	0.03	-5.27	-2.38	CRTVQPATPVANQP	802.3	3.4
		quebec-11	0.155	0.021	3.16	0.01	-5.90	-2.29	KIOCHYWMUMWWKS	861.2	3.4
		quebec-12	0.136	0.029	2.86	0.02	-6.33	-3.10	XNPDXMLQECTYDD	924.2	4.0

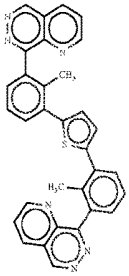
FIGURE 91



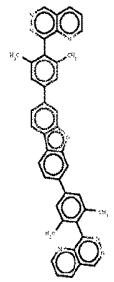
Nickname	quebec-1
Splitting	0.141 (eV)
Strength	0.035
Absorption	2.90 (eV)
Rate	0.02 (1/ns)
HOMO	-5.56 (eV)
LUMO	-2.21 (eV)
Key	NAOLMGTWCVCQLN
Weight	427.17
SA Score	2.63
Color Est.:	



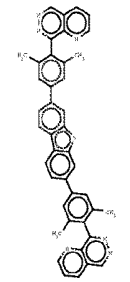
Nickname	quebec-2
Splitting	0.166 (eV)
Strength	0.012
Absorption	2.84 (eV)
Rate	0.00 (1/ns)
HOMO	-5.66 (eV)
LUMO	-2.42 (eV)
Key	HOHSBCOUWGWHSN
Weight	522.16
SA Score	3.05
Color Est.:	



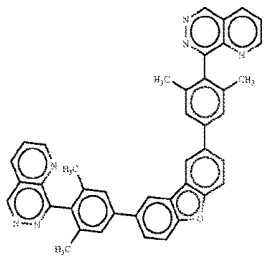
Nickname	quebec-3
Splitting	0.116 (eV)
Strength	0.036
Absorption	2.79 (eV)
Rate	0.05 (1/ns)
HOMO	-5.37 (eV)
LUMO	-2.17 (eV)
Key	JYQURBPZOYNSHP
Weight	522.16
SA Score	3.10
Color Est.:	



Nickname	quebec-5
Splitting	0.135 (eV)
Strength	0.075
Absorption	2.81 (eV)
Rate	0.05 (1/ns)
HOMO	-5.40 (eV)
LUMO	-2.21 (eV)
Key	FEAWYSMGXAAHEH
Weight	634.25
SA Score	3.26
Color Est.:	



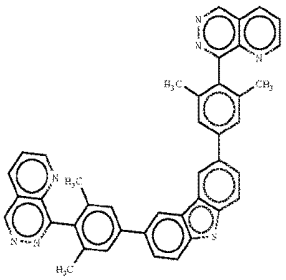
Nickname	quebec-6
Splitting	0.169 (eV)
Strength	0.098
Absorption	2.85 (eV)
Rate	0.02 (1/ns)
HOMO	-5.44 (eV)
LUMO	-2.21 (eV)
Key	SJYRYFHHVZQOKN
Weight	650.23
SA Score	3.28
Color Est.:	



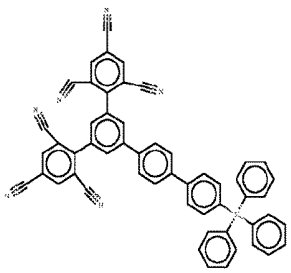
Nickname	quebec-7
Splitting	0.155 (eV)
Strength	0.047
Absorption	2.94 (eV)
Rate	0.01 (1/ns)
HOMO	-5.57 (eV)
LUMO	-2.19 (eV)
Key	YYDAGVMGKQCLNP
Weight	634.25
SA Score	3.24
Color Est.:	

Table 8

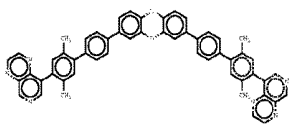
FIGURE 92



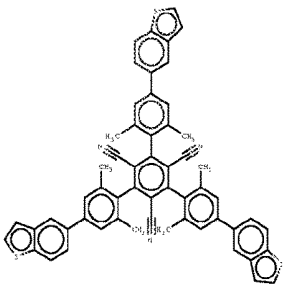
Nickname	quebec-8
Splitting	0.085 (eV)
Strength	0.027
Absorption	2.83 (eV)
Rate	0.12 (1/us)
HOMO	-5.42 (eV)
LUMO	-2.23 (eV)
Key	LVWRADBSUWLHOE
Weight	650.23
SA Score	3.27
Color Est.:	



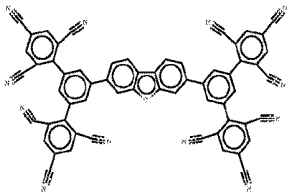
Nickname	quebec-9
Splitting	0.120 (eV)
Strength	0.016
Absorption	2.81 (eV)
Rate	0.02 (1/us)
HOMO	-6.22 (eV)
LUMO	-3.02 (eV)
Key	COWVQULBZVWOPZ
Weight	790.23
SA Score	3.28
Color Est.:	



Nickname	quebec-10
Splitting	0.090 (eV)
Strength	0.010
Absorption	2.69 (eV)
Rate	0.03 (1/us)
HOMO	-5.27 (eV)
LUMO	-2.38 (eV)
Key	CRTVQPATPVANQP
Weight	802.31
SA Score	3.35
Color Est.:	



Nickname	quebec-11
Splitting	0.155 (eV)
Strength	0.021
Absorption	3.16 (eV)
Rate	0.01 (1/us)
HOMO	-5.90 (eV)
LUMO	-2.29 (eV)
Key	KIOCHYWMUMWWKS
Weight	861.23
SA Score	3.44
Color Est.:	



Nickname	quebec-12
Splitting	0.136 (eV)
Strength	0.029
Absorption	2.86 (eV)
Rate	0.02 (1/us)
HOMO	-6.33 (eV)
LUMO	-3.10 (eV)
Key	XNPDXMLQECTYDD
Weight	924.19
SA Score	3.98
Color Est.:	

FIGURE 93

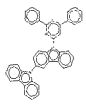
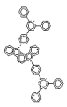
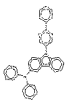
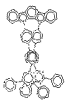
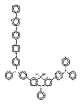
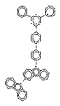
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
			0.113	0.045	3.07	0.08	-5.19	-1.77	FFVHDJGQAYZBAF	562.2	2.4
			0.196	0.211	2.90	0.01	-5.11	-1.81	WLKYYCHHBJEQAB	868.3	3.0
			0.183	0.126	2.84	0.01	-4.83	-1.60	XCTSVTLGQCWKKS	488.2	2.4
			0.202	0.057	2.93	0.00	-5.16	-1.90	CRELPLJMKYUMQO	1020.4	3.2
			0.217	0.256	2.91	0.01	-4.99	-1.78	QXCYAUDLEJUDJD	868.3	2.9
			0.224	0.260	2.76	0.00	-4.60	-1.67	DSWZOBDTWBODKE	1077.5	3.5
			0.217	0.090	3.01	0.00	-5.15	-1.90	RBFYESZIZZZDEO	714.3	2.5

Table 9

FIGURE 94

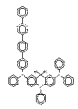
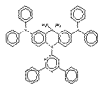
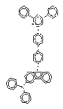
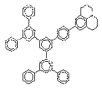
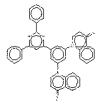
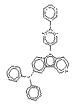
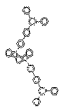
Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
			0.224	0.308	2.67	0.01	-4.48	-1.58	ALVVLHYMRFHFDE	849.4	3.0
			0.210	0.041	3.09	0.00	-4.84	-1.32	MEHXCDLDGNGYCR	773.4	3.0
			0.184	0.124	2.90	0.01	-4.93	-1.78	VRIVSVIGPHYONT	717.3	2.8
			0.145	0.025	2.81	0.01	-4.68	-1.61	UNHOPSDNMWYNFS	785.4	2.8
			0.125	0.032	3.07	0.03	-5.90	-2.33	UFUKENCATKAJKL	594.2	2.7
			0.140	0.087	2.85	0.05	-4.97	-1.74	YIMDVNNSMZOUMV	489.2	2.5
			0.191	0.107	2.92	0.01	-5.06	-1.84	FOLVSJICFOFVKS	1020.4	3.3

FIGURE 95

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
			0.210	0.046	2.86	0.00	-4.72	-1.64	JATNYGNICJOTGS	1098.4	3.5
			0.221	0.027	3.03	0.00	-5.42	-1.98	NHMQSLHGRPOGCE	524.2	2.4
			0.214	0.067	2.90	0.00	-4.82	-1.72	UEIWSWXBMQTVIF	868.4	2.9
			0.208	0.204	2.78	0.01	-4.75	-1.59	UPLPGMCFTKMOAN	655.3	2.6
			0.197	0.029	3.09	0.00	-5.48	-1.92	AWYIEKAQFCMGSP	538.2	2.5
			0.123	0.028	2.71	0.02	-4.45	-1.48	DEMMSGJIBMDTFE	1080.4	3.7
		lima8-19	0.084	0.087	2.75	0.36	-4.80	-1.84	OUIBDFADJBVHAC	792.3	2.8

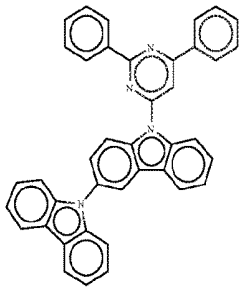
FIGURE 96

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		lima17-36	0.180	0.257	2.81	0.03	-5.02	-1.83	AQKHOZSZROSAFH	868.3	2.9
		lima17-37	0.184	0.230	2.90	0.02	-4.84	-1.71	MUWFERWTYXSXGE	1020.4	3.2
		lima17-38	0.148	0.217	2.82	0.08	-4.96	-1.84	WRVHMDICBYATEF	1020.4	3.2
		lima29-68	0.121	0.183	2.70	0.18	-4.78	-1.81	CGHHQAFAECWPKU	959.4	3.1
		lima29-71	0.087	0.135	2.70	0.49	-4.76	-1.85	WQNAHZHSXRCFTB	1035.4	3.2
		lima30-72	0.124	0.154	2.79	0.15	-4.78	-1.77	DLVCLJKTJWLZGG	959.4	3.1
		lima33-84	0.146	0.186	2.80	0.08	-4.80	-1.74	IONWQDMTUKFFPS	883.4	2.9

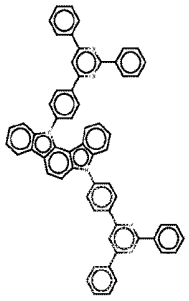
FIGURE 97

Color	Structure	Name	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
		mike17-38	0.123	0.188	2.65	0.16	-4.70	-1.75	YPEPVXACQYSHHX	731.3	2.7
		mike34-91	0.105	0.102	2.68	0.17	-4.59	-1.72	DFUKIZSMGVMUNC	883.4	3.0
		november13-15	0.117	0.060	2.85	0.08	-4.81	-1.66	JIKPBZAYXVCJFJ	883.4	3.0
		november44-58	0.099	0.084	2.81	0.21	-4.89	-1.83	TWCHSQCJSKLHHZ	641.3	2.7
		november64-90	0.132	0.059	3.01	0.05	-5.29	-1.99	NIHCWPMKEHXHCQ	639.2	2.7
		november84-116	0.108	0.112	2.74	0.18	-4.78	-1.74	VYQIYBTZPUGCBC	564.2	2.5
		november105-143	0.115	0.092	2.76	0.12	-4.67	-1.71	ZXTMKRLDMGSHKT	716.3	2.6

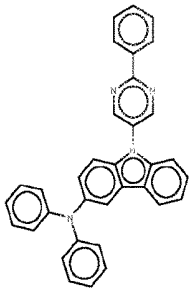
FIGURE 98



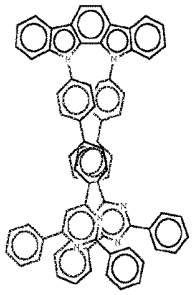
Nickname	
Splitting	0.113 (eV)
Strength	0.045
Absorption	3.07 (eV)
Rate	0.08 (1/ns)
HOMO	-5.19 (eV)
LUMO	-1.77 (eV)
Key	FFVHDJGQAYZBAF
Weight	562.22
SA Score	2.40
Color Est.:	



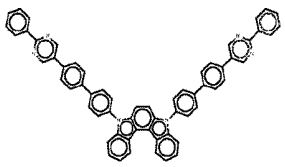
Nickname	
Splitting	0.196 (eV)
Strength	0.211
Absorption	2.90 (eV)
Rate	0.01 (1/ns)
HOMO	-5.11 (eV)
LUMO	-1.81 (eV)
Key	WLKYYCHHBJEQAB
Weight	868.33
SA Score	2.98
Color Est.:	



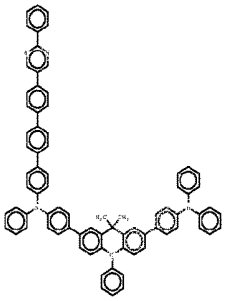
Nickname	
Splitting	0.183 (eV)
Strength	0.126
Absorption	2.84 (eV)
Rate	0.01 (1/ns)
HOMO	-4.83 (eV)
LUMO	-1.60 (eV)
Key	XCTSVTLGQCWKKS
Weight	488.20
SA Score	2.38
Color Est.:	



Nickname	
Splitting	0.202 (eV)
Strength	0.057
Absorption	2.93 (eV)
Rate	0.00 (1/ns)
HOMO	-5.16 (eV)
LUMO	-1.90 (eV)
Key	CRELRLJMKYUMQO
Weight	1020.39
SA Score	3.18
Color Est.:	



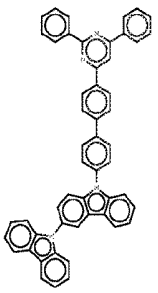
Nickname	
Splitting	0.217 (eV)
Strength	0.256
Absorption	2.91 (eV)
Rate	0.01 (1/ns)
HOMO	-4.99 (eV)
LUMO	-1.78 (eV)
Key	QXCYAUDLEJUDJD
Weight	868.33
SA Score	2.88
Color Est.:	



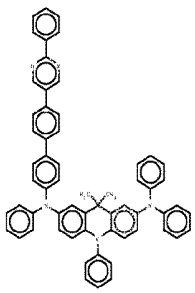
Nickname	
Splitting	0.224 (eV)
Strength	0.260
Absorption	2.76 (eV)
Rate	0.00 (1/ns)
HOMO	-4.60 (eV)
LUMO	-1.67 (eV)
Key	DSWZORDTWBODKE
Weight	1077.48
SA Score	3.46
Color Est.:	

Table 10

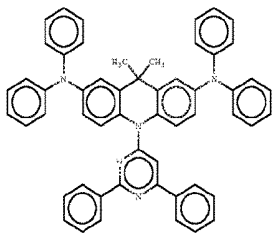
FIGURE 99



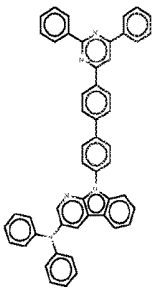
Nickname	
Splitting	0.217 (eV)
Strength	0.090
Absorption	3.01 (eV)
Rate	0.00 (1/us)
HOMO	-5.15 (eV)
LUMO	-1.90 (eV)
Key	RBFYESZIZZZDEO
Weight	714.28
SA Score	2.52
Color Est.:	



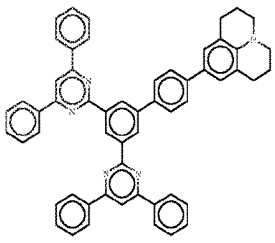
Nickname	
Splitting	0.224 (eV)
Strength	0.308
Absorption	2.67 (eV)
Rate	0.01 (1/us)
HOMO	-4.48 (eV)
LUMO	-1.58 (eV)
Key	ALVVLHYMRFHEDE
Weight	849.38
SA Score	3.05
Color Est.:	



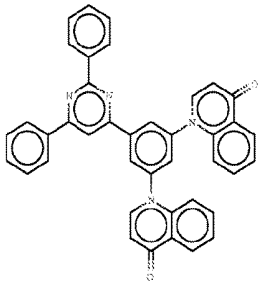
Nickname	
Splitting	0.210 (eV)
Strength	0.041
Absorption	3.09 (eV)
Rate	0.00 (1/us)
HOMO	-4.84 (eV)
LUMO	-1.32 (eV)
Key	MEHXCDLDGNGYCR
Weight	773.35
SA Score	2.96
Color Est.:	



Nickname	
Splitting	0.184 (eV)
Strength	0.124
Absorption	2.90 (eV)
Rate	0.01 (1/us)
HOMO	-4.93 (eV)
LUMO	-1.78 (eV)
Key	VBIVSVIGPHYONT
Weight	717.29
SA Score	2.80
Color Est.:	

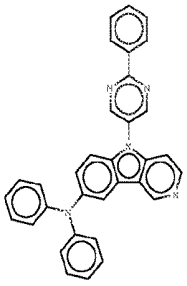


Nickname	
Splitting	0.145 (eV)
Strength	0.025
Absorption	2.81 (eV)
Rate	0.01 (1/us)
HOMO	-4.68 (eV)
LUMO	-1.61 (eV)
Key	UNHOPSDNMWYNFS
Weight	785.35
SA Score	2.83
Color Est.:	

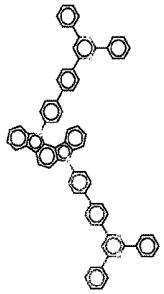


Nickname	
Splitting	0.125 (eV)
Strength	0.032
Absorption	3.07 (eV)
Rate	0.03 (1/us)
HOMO	-5.90 (eV)
LUMO	-2.33 (eV)
Key	UFUKENCATKAJKL
Weight	594.21
SA Score	2.73
Color Est.:	

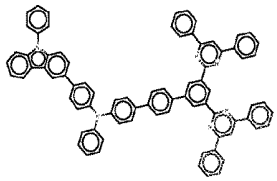
FIGURE 100



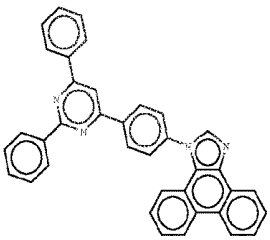
Nickname	
Splitting	0.140 (eV)
Strength	0.087
Absorption	2.85 (eV)
Rate	0.05 (1/ns)
HOMO	-4.97 (eV)
LUMO	-1.74 (eV)
Key	YBMDVNNSMZOUMV
Weight	489.20
SA Score	2.53
Color Est.:	



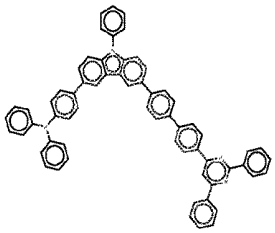
Nickname	
Splitting	0.191 (eV)
Strength	0.107
Absorption	2.92 (eV)
Rate	0.01 (1/ns)
HOMO	-5.06 (eV)
LUMO	-1.84 (eV)
Key	FOLVSJICFOFVKS
Weight	1020.39
SA Score	3.28
Color Est.:	



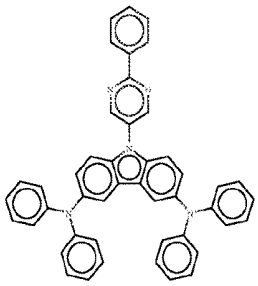
Nickname	
Splitting	0.210 (eV)
Strength	0.046
Absorption	2.86 (eV)
Rate	0.00 (1/ns)
HOMO	-4.72 (eV)
LUMO	-1.64 (eV)
Key	JATNYGNICJOTGS
Weight	1098.44
SA Score	3.50
Color Est.:	



Nickname	
Splitting	0.221 (eV)
Strength	0.027
Absorption	3.03 (eV)
Rate	0.00 (1/ns)
HOMO	-5.42 (eV)
LUMO	-1.98 (eV)
Key	NEMQSLHGRPOGCE
Weight	524.20
SA Score	2.40
Color Est.:	

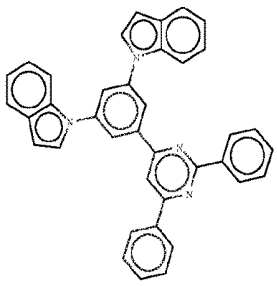


Nickname	
Splitting	0.214 (eV)
Strength	0.067
Absorption	2.90 (eV)
Rate	0.00 (1/ns)
HOMO	-4.82 (eV)
LUMO	-1.72 (eV)
Key	UEWSWXBMQTVIF
Weight	868.36
SA Score	2.85
Color Est.:	

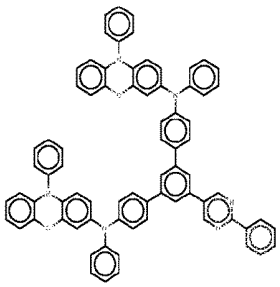


Nickname	
Splitting	0.208 (eV)
Strength	0.204
Absorption	2.78 (eV)
Rate	0.01 (1/ns)
HOMO	-4.75 (eV)
LUMO	-1.59 (eV)
Key	UPLPGMCFTKMOAN
Weight	655.27
SA Score	2.59
Color Est.:	

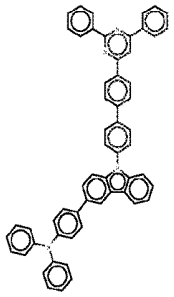
FIGURE 101



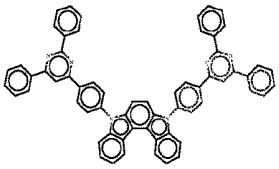
Nickname	
Splitting	0.197 (eV)
Strength	0.029
Absorption	3.09 (eV)
Rate	0.00 (1/ns)
HOMO	-5.48 (eV)
LUMO	-1.92 (eV)
Key	AWYHKAQFCMGSP
Weight	538.22
SA Score	2.52
Color Est.:	



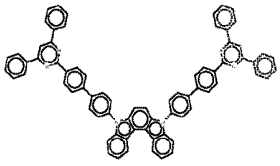
Nickname	
Splitting	0.123 (eV)
Strength	0.028
Absorption	2.71 (eV)
Rate	0.02 (1/ns)
HOMO	-4.45 (eV)
LUMO	-1.48 (eV)
Key	DEMMSGJBMDTFE
Weight	1080.42
SA Score	3.66
Color Est.:	



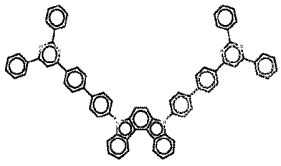
Nickname	lima8-19
Splitting	0.084 (eV)
Strength	0.087
Absorption	2.75 (eV)
Rate	0.36 (1/ns)
HOMO	-4.80 (eV)
LUMO	-1.84 (eV)
Key	OUIBDFADJBVHAC
Weight	792.33
SA Score	2.75
Color Est.:	



Nickname	lima17-36
Splitting	0.180 (eV)
Strength	0.257
Absorption	2.81 (eV)
Rate	0.03 (1/ns)
HOMO	-5.02 (eV)
LUMO	-1.83 (eV)
Key	AQKHOZSZROSAFH
Weight	868.33
SA Score	2.89
Color Est.:	

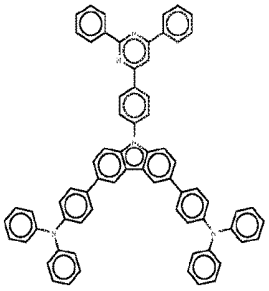


Nickname	lima17-37
Splitting	0.184 (eV)
Strength	0.230
Absorption	2.90 (eV)
Rate	0.02 (1/ns)
HOMO	-4.84 (eV)
LUMO	-1.71 (eV)
Key	MUWFERWTYXSXGE
Weight	1020.39
SA Score	3.18
Color Est.:	

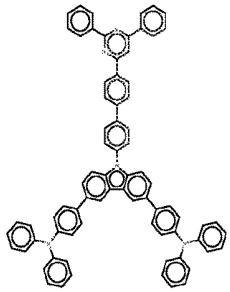


Nickname	lima17-38
Splitting	0.148 (eV)
Strength	0.217
Absorption	2.82 (eV)
Rate	0.08 (1/ns)
HOMO	-4.96 (eV)
LUMO	-1.84 (eV)
Key	WRVHMDICBYATDF
Weight	1020.39
SA Score	3.18
Color Est.:	

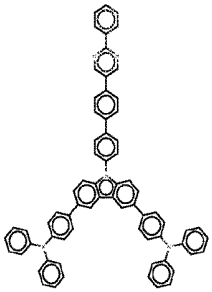
FIGURE 102



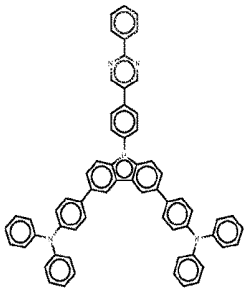
Nickname	lima29-68
Splitting	0.121 (eV)
Strength	0.183
Absorption	2.70 (eV)
Rate	0.18 (1/ns)
HOMO	-4.78 (eV)
LUMO	-1.81 (eV)
Key	CGHHQAFAECWPKU
Weight	959.40
SA Score	3.09
Color Est.:	



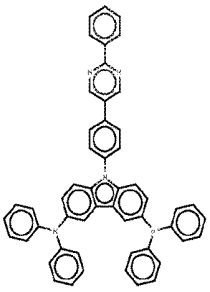
Nickname	lima29-71
Splitting	0.087 (eV)
Strength	0.135
Absorption	2.70 (eV)
Rate	0.49 (1/ns)
HOMO	-4.76 (eV)
LUMO	-1.85 (eV)
Key	WQNAHZHSXRCFTB
Weight	1035.43
SA Score	3.24
Color Est.:	



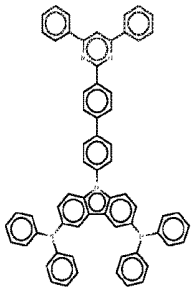
Nickname	lima30-72
Splitting	0.124 (eV)
Strength	0.154
Absorption	2.79 (eV)
Rate	0.15 (1/ns)
HOMO	-4.78 (eV)
LUMO	-1.77 (eV)
Key	DLVCLJKTJWLZGG
Weight	959.40
SA Score	3.08
Color Est.:	



Nickname	lima33-84
Splitting	0.146 (eV)
Strength	0.186
Absorption	2.80 (eV)
Rate	0.08 (1/ns)
HOMO	-4.80 (eV)
LUMO	-1.74 (eV)
Key	IONWQDMTUKFPFS
Weight	883.37
SA Score	2.94
Color Est.:	

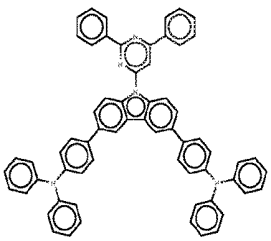


Nickname	mike17-38
Splitting	0.123 (eV)
Strength	0.188
Absorption	2.65 (eV)
Rate	0.16 (1/ns)
HOMO	-4.70 (eV)
LUMO	-1.75 (eV)
Key	YPEPVXACQYSBEX
Weight	731.30
SA Score	2.72
Color Est.:	

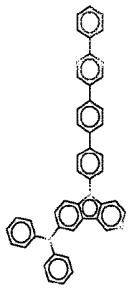


Nickname	mike34-91
Splitting	0.105 (eV)
Strength	0.102
Absorption	2.68 (eV)
Rate	0.17 (1/ns)
HOMO	-4.59 (eV)
LUMO	-1.72 (eV)
Key	DFUKIZSMGVMUNC
Weight	883.37
SA Score	2.96
Color Est.:	

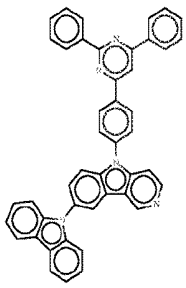
FIGURE 103



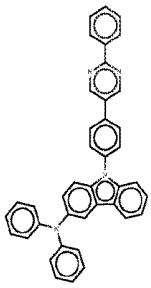
Nickname	november13-15
Splitting	0.117 (eV)
Strength	0.060
Absorption	2.85 (eV)
Rate	0.08 (1/ns)
HOMO	-4.81 (eV)
LUMO	-1.66 (eV)
Key	JBKPBZAYXVCJFJ
Weight	883.37
SA Score	2.97
Color Est.:	



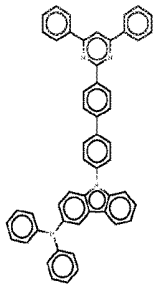
Nickname	november44-58
Splitting	0.099 (eV)
Strength	0.084
Absorption	2.81 (eV)
Rate	0.21 (1/ns)
HOMO	-4.89 (eV)
LUMO	-1.83 (eV)
Key	TWCHSQCJSKLHHZ
Weight	641.26
SA Score	2.71
Color Est.:	



Nickname	november64-90
Splitting	0.132 (eV)
Strength	0.059
Absorption	3.01 (eV)
Rate	0.05 (1/ns)
HOMO	-5.29 (eV)
LUMO	-1.99 (eV)
Key	NIHCWPMKEHNHCQ
Weight	639.24
SA Score	2.65
Color Est.:	



Nickname	november84-116
Splitting	0.108 (eV)
Strength	0.112
Absorption	2.74 (eV)
Rate	0.18 (1/ns)
HOMO	-4.78 (eV)
LUMO	-1.74 (eV)
Key	VYQHYBTZPUGCBC
Weight	564.23
SA Score	2.46
Color Est.:	



Nickname	november105-143
Splitting	0.115 (eV)
Strength	0.092
Absorption	2.76 (eV)
Rate	0.12 (1/ns)
HOMO	-4.67 (eV)
LUMO	-1.71 (eV)
Key	ZXTMKRLDMGSHKT
Weight	716.29
SA Score	2.64
Color Est.:	

FIGURE 104

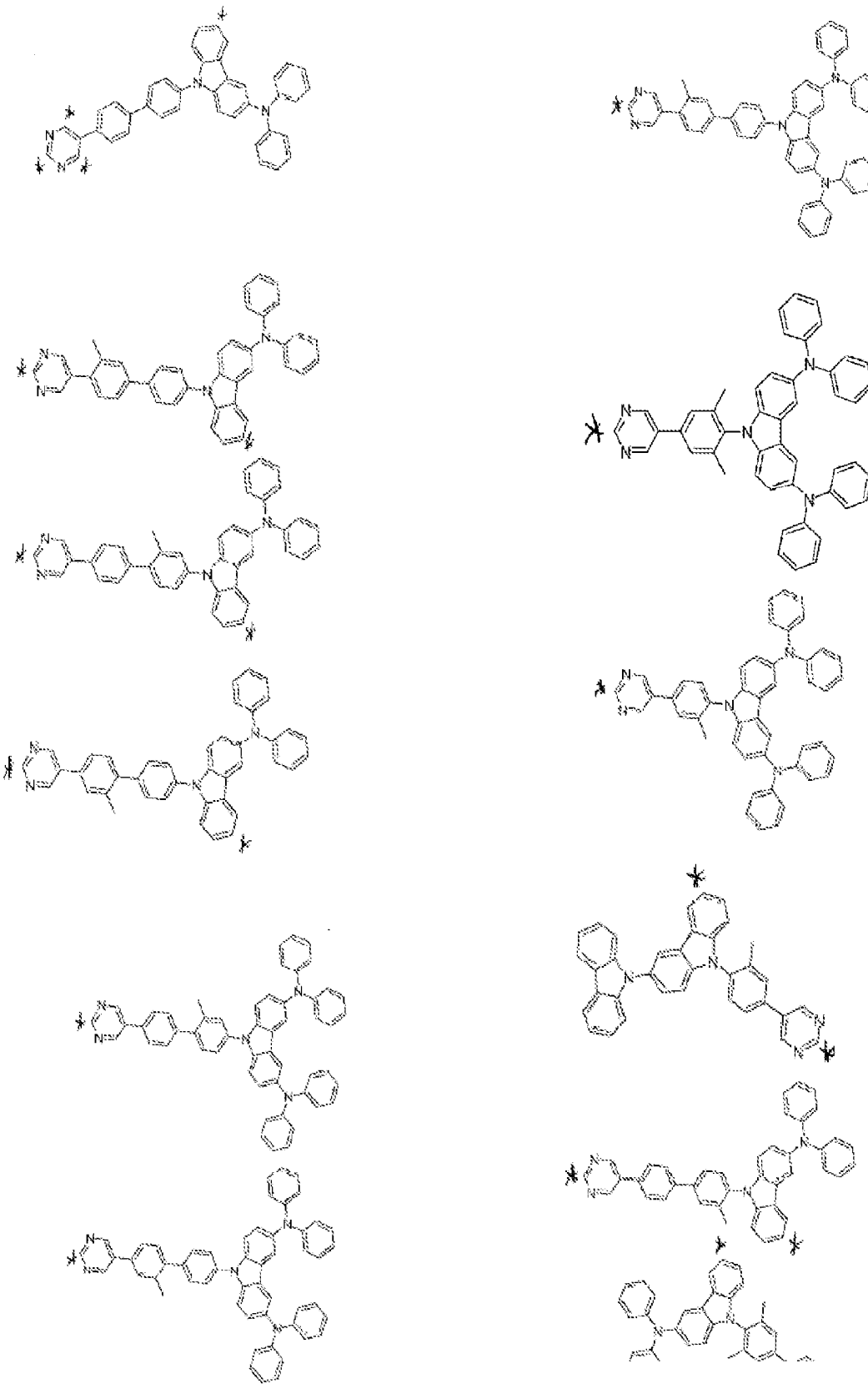


Table 11

FIGURE 105

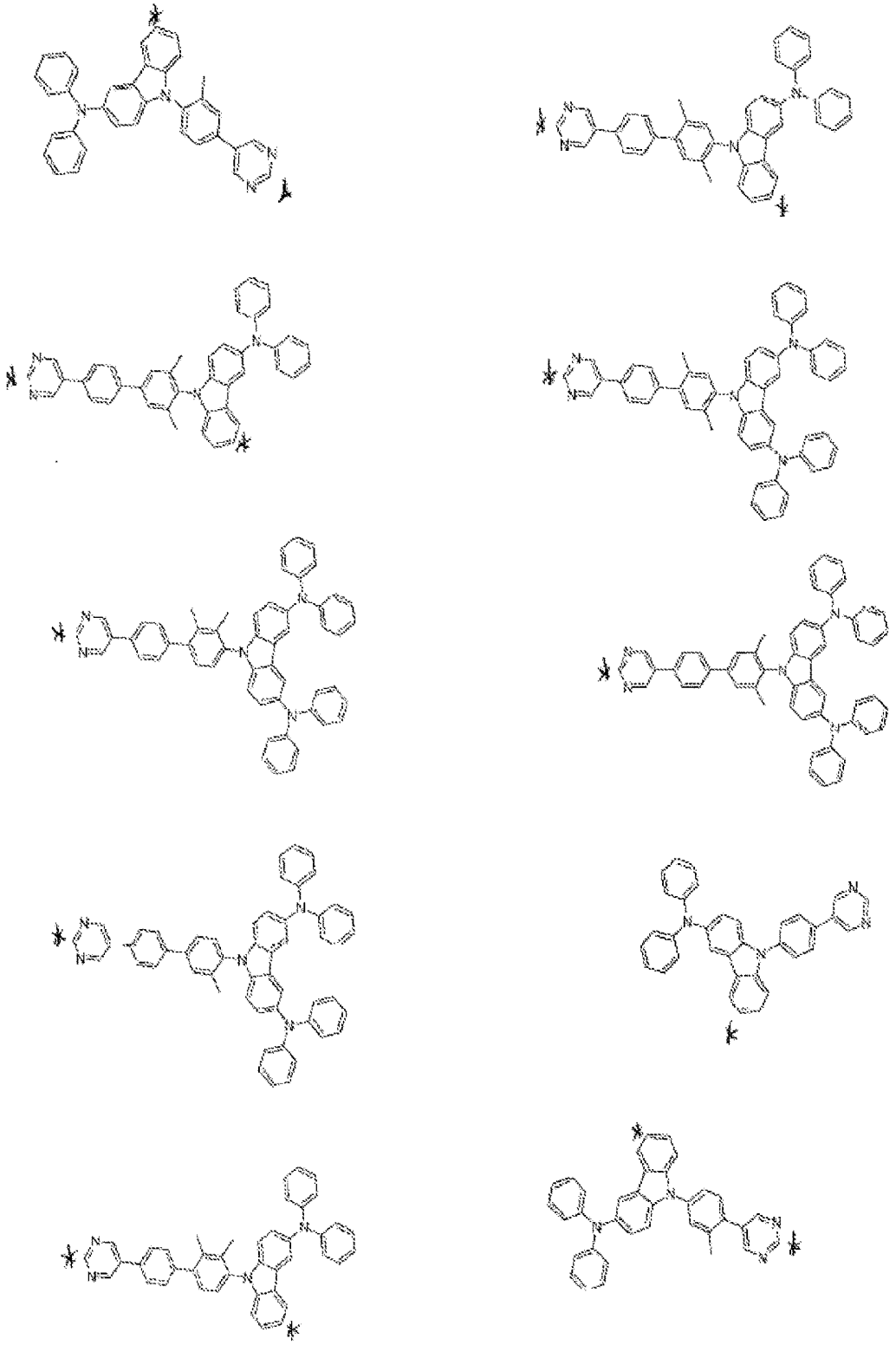


FIGURE 106

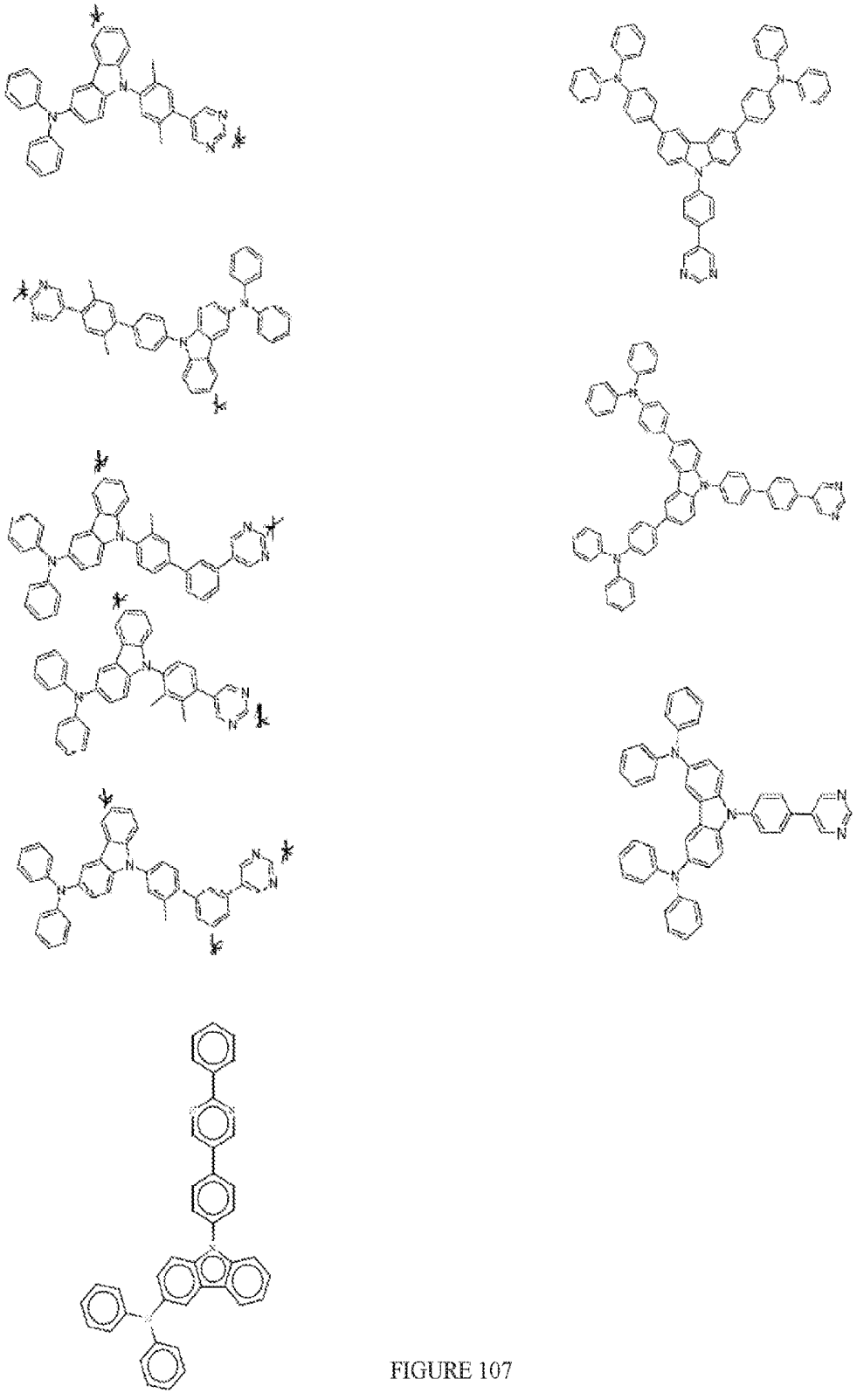


FIGURE 107

Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
echo_prime-6,romeo_53-116		S1		0.225	0.004	3.15	0.00	-5.25	-1.55	HEEAVJOEDUPPBL	590.2	3.0
		T1		0.151	0.011	2.87	0.00					
india1-32-1,romeo_52-114		S1		0.125	0.031	2.74	0.03	-5.40	-2.09	IJKPZGOXGBSTOR	512.2	2.7
		T1		0.092	0.008	2.43	0.02					
romeo_1-1		S1		0.081	0.007	2.78	0.03	-4.80	-1.59	UZFCMYUNYYFGID	1020.4	3.4
		T1		0.136	0.008	2.54	0.01					
romeo_3-4		S1		0.078	0.004	2.84	0.02	-5.20	-1.94	CFYSESBGRZNWCY	1024.4	3.4
		T1		0.157	0.005	2.60	0.00					
romeo_4-5		S1		0.073	0.004	2.62	0.03	-5.70	-2.65	PPAJVSSPIIVUCJ	1256.4	4.6
		T1		0.069	0.011	2.07	0.05					
romeo_4-6		S1		0.102	0.004	2.86	0.01	-5.33	-1.97	LCPMSDXWMZKSMD	984.3	3.6
		T1		0.120	0.018	2.55	0.02					
romeo_5-8		S1		0.284	0.106	2.78	0.00	-5.24	-1.99	WLTPAHYVIWLZMH	512.2	2.8
		T1		0.204	0.114	2.41	0.00					
romeo_5-10		S1		0.024	0.018	2.76	0.70	-4.88	-1.91	QEOYGOOUEAGYLH	872.4	3.4
		T1		0.172	0.017	2.59	0.00					

Table 12

FIGURE 108

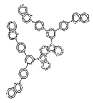
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_5-11		S1		0.081	0.007	2.57	0.03	-5.24	-2.13	LWHLTOWXFCGGLI	512.2	2.8
		T1		0.076	0.005	2.28	0.02					
romeo_5-12		S1		0.086	0.006	2.64	0.02	-5.03	-2.10	HJGPOCLOABFFMU	1224.4	4.2
		T1		0.026	0.007	2.41	0.20					
romeo_5-13		S1		0.043	0.004	2.48	0.07	-4.88	-2.02	YSXJFOPCWOIRJW	664.2	3.0
		T1		0.181	0.003	2.07	0.00					
romeo_5-14		S1		0.062	0.004	2.77	0.04	-5.25	-2.12	OUCKBNNSNFIAMH	920.3	3.6
		T1		0.086	0.002	2.54	0.00					
romeo_5-15		S1		0.114	0.004	2.70	0.00	-4.95	-1.99	UNTSBCJGYFZYRP	872.4	3.4
		T1		0.102	0.002	2.49	0.00					
romeo_5-16		S1		0.072	0.003	2.80	0.02	-5.01	-1.88	UXYQODLZQANYBW	748.3	3.5
		T1		0.223	0.004	2.61	0.00					
romeo_5-17		S1		0.103	0.003	2.67	0.01	-4.96	-2.02	PNOQAAQFAGGPTH	816.3	3.2
		T1		0.029	0.003	2.45	0.08					
romeo_6-19		S1		0.040	0.006	2.71	0.14	-5.07	-2.00	KEOVYHKYXHKQAB	1128.4	3.4
		T1		0.042	0.004	2.45	0.06					

FIGURE 109

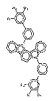
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_6-20		S1		0.024	0.006	2.67	0.22	-5.04	-2.10	HXRJEQIWVKWFCG	1432.5	4.1
		T1		0.038	0.005	2.45	0.12					
romeo_6-21		S1		0.056	0.003	2.81	0.04	-4.96	-1.90	QEOOAVVYJLBMDN	920.3	2.9
		T1		0.198	0.003	2.61	0.00					
romeo_7-22		S1		0.107	0.073	2.52	0.11	-4.82	-1.99	BWRVADAAULZSQQ	664.2	2.9
		T1		0.078	0.072	2.28	0.26					
romeo_7-24		S1		0.048	0.004	2.62	0.06	-4.81	-1.93	FWRRZOOXQACFJG	1224.4	4.2
		T1		0.010	0.004	2.40	0.16					
romeo_8-26		S1		0.069	0.004	2.84	0.03	-5.41	-2.16	OJRNSZGVPSGNNL	968.1	3.6
		T1		0.194	0.002	2.66	0.00					
romeo_9-27		S1		0.142	0.004	2.89	0.00	-5.44	-2.07	ZXTDGXPCSHOIDY	968.1	3.1
		T1		0.114	0.006	2.52	0.01					
romeo_11-29		S1		0.118	0.115	2.60	0.12	-4.92	-1.98	JCAIMPUPRNOMAE	664.2	2.8
		T1		0.097	0.108	2.37	0.21					
romeo_11-31		S1		0.175	0.076	2.48	0.01	-5.02	-2.02	DWZQOAQTEUJMNH	512.2	2.7
		T1		0.136	0.069	2.03	0.02					

FIGURE 110

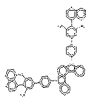
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_11-32		S1		0.005	0.007	2.74	0.48	-4.81	-1.86	ZBBQWXUUNMUQIV	872.4	3.4
		T1		0.171	0.003	2.58	0.00					
romeo_11-33		S1		0.033	0.006	2.45	0.13	-4.86	-2.02	NZNIAHPLMALOMN	920.3	3.6
		T1		0.031	0.008	2.17	0.14					
romeo_11-34		S1		0.005	0.003	2.69	0.20	-4.84	-1.90	YTSUUEFNJKPPSB	900.4	3.6
		T1		0.103	0.003	2.49	0.00					
romeo_12-35		S1		0.106	0.008	2.72	0.01	-5.15	-1.93	FDFPXBXNVGEMMW	876.3	3.4
		T1		0.162	0.011	2.45	0.00					
romeo_13-36		S1		0.206	0.105	2.93	0.01	-5.26	-1.87	HVGIEKZUMDTYIS	718.3	3.0
		T1		0.193	0.105	2.49	0.01					
romeo_14-37		S1		0.062	0.006	2.76	0.06	-5.04	-1.98	WVUHNKXRXZUYQY	1224.4	4.2
		T1		0.015	0.004	2.51	0.16					
romeo_15-38		S1		0.098	0.003	2.71	0.01	-5.27	-2.06	DOTRMYMFDRYGGE	824.3	2.8
		T1		0.160	0.003	2.18	0.00					
romeo_16-40		S1		0.049	0.042	2.74	0.66	-4.90	-1.91	DAHMLXBTBYGJQW	848.3	3.1
		T1		0.171	0.039	2.58	0.01					

FIGURE 111

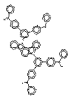
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_16-41		S1		0.130	0.074	2.66	0.05	-5.66	-2.63	ILBJEVDOPZJFPI	554.1	3.2
		T1		0.135	0.062	2.10	0.02					
romeo_16-42		S1		0.074	0.033	2.68	0.19	-4.89	-1.81	CCLXRXILXXYWAA	660.2	3.1
		T1		0.133	0.029	2.46	0.08					
romeo_17-43		S1		0.053	0.010	2.84	0.14	-5.23	-2.02	YNZDDDBGQQVYSS	1128.4	3.5
		T1		0.030	0.005	2.55	0.14					
romeo_17-44		S1		0.056	0.004	2.61	0.05	-5.19	-2.11	KSPQBHPCLDCQKM	824.3	2.9
		T1		0.079	0.009	2.27	0.03					
romeo_18-45		S1		0.154	0.008	2.78	0.00	-5.04	-1.70	MCWZEFNWYBAIMO	510.2	2.6
		T1		0.145	0.004	2.55	0.00					
romeo_19-46		S1		0.183	0.241	2.79	0.02	-5.06	-1.93	IOYAUPBJEGJNLP	848.3	2.9
		T1		0.209	0.225	2.61	0.01					
romeo_19-47		S1		0.171	0.217	2.77	0.03	-5.09	-1.99	XJUWMLPOYFEFDR	696.2	2.9
		T1		0.141	0.204	2.57	0.09					
romeo_19-48		S1		0.044	0.008	2.66	0.14	-5.22	-2.17	WNNJYSJOWGNEHT	984.3	3.8
		T1		0.046	0.012	2.39	0.16					

FIGURE 112

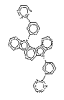
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_19-49		S1		0.064	0.004	2.72	0.03	-4.90	-1.78	BHWAECORJNUTMY	984.3	3.4
		T1		0.061	0.001	2.48	0.01					
romeo_19-50		S1		0.062	0.003	2.76	0.03	-5.04	-1.92	CFDMJGMJSNUEO	848.3	3.0
		T1		0.122	0.004	2.55	0.00					
romeo_19-51		S1		0.051	0.003	2.78	0.04	-5.10	-1.93	IFRWBFBCKLFFJA	1096.4	4.4
		T1		0.109	0.005	2.54	0.01					
romeo_20-52		S1		0.056	0.012	2.73	0.14	-4.91	-1.76	XKTRDQHKHTXDJM	812.3	3.1
		T1		0.056	0.016	2.47	0.15					
romeo_20-53		S1		0.055	0.009	2.80	0.12	-5.23	-2.07	AKNFYTRLBFKUMU	1116.4	3.5
		T1		0.164	0.009	2.60	0.00					
romeo_20-54		S1		0.043	0.005	2.72	0.10	-4.77	-1.64	APIMRUSOUHQFFK	610.2	2.7
		T1		0.086	0.006	2.50	0.03					
romeo_20-55		S1		0.063	0.004	2.79	0.03	-5.41	-2.19	YINDVOQEHGNQQV	812.3	3.0
		T1		0.098	0.010	2.55	0.03					
romeo_21-56		S1		0.095	0.013	2.84	0.04	-4.89	-1.59	YUDUNOGIJFJJRC	584.2	2.7
		T1		0.054	0.008	2.55	0.09					

FIGURE 113

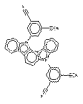
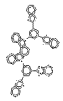
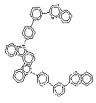
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_22-57		S1		0.099	0.003	2.78	0.01	-5.85	-2.53	MTIQVDHNSNHQQU	508.1	2.9
		T1		0.028	0.006	2.32	0.14					
romeo_24-59		S1		0.082	0.008	2.59	0.03	-4.70	-1.65	UOWUJTBPHSXYSU	720.3	3.0
		T1		0.054	0.003	2.30	0.02					
romeo_24-60		S1		0.087	0.004	2.79	0.02	-4.65	-1.40	FLAFWVVWKWBXLT	748.3	3.3
		T1		0.135	0.002	2.54	0.00					
romeo_24-61		S1		0.095	0.004	2.76	0.01	-4.78	-1.57	GVOBIALXPLREAQ	564.2	2.6
		T1		0.121	0.001	2.58	0.00					
romeo_25-62		S1		0.093	0.004	2.62	0.01	-5.01	-1.91	ZFSSPCXZVBPNOY	876.3	3.3
		T1		0.074	0.008	2.30	0.03					
romeo_26-63		S1		0.124	0.089	2.51	0.07	-5.00	-2.09	ZJRPMXYZEWDXGL	664.2	2.7
		T1		0.085	0.085	2.41	0.26					
romeo_26-65		S1		0.042	0.004	2.61	0.08	-4.93	-2.07	OEYUJUMCLBPITA	816.3	3.0
		T1		0.015	0.005	2.41	0.19					
romeo_27-66		S1		0.157	0.120	2.65	0.03	-4.83	-1.94	BCVXLCIGGAYVPB	816.3	2.9
		T1		0.094	0.112	2.47	0.29					

FIGURE 114

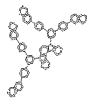
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_27-67		S1		0.181	0.089	2.78	0.01	-5.10	-2.00	CXZMGPRYZWWSOT	664.2	2.8
		T1		0.178	0.089	2.61	0.01					
romeo_27-68		S1		0.206	0.039	2.70	0.00	-5.26	-2.09	SVUZZOHTVCTEIB	512.2	2.8
		T1		0.134	0.016	2.41	0.01					
romeo_27-69		S1		0.042	0.008	2.62	0.15	-4.79	-1.92	FOTLQCCOOKORJG	816.3	3.0
		T1		0.043	0.007	2.45	0.10					
romeo_27-70		S1		0.135	0.007	2.81	0.00	-5.14	-2.04	AOKUWYWDUTVRBL	1224.4	4.1
		T1		0.176	0.006	2.61	0.00					
romeo_27-71		S1		0.164	0.006	2.80	0.00	-4.85	-1.84	RMAUFCQUYIHJQB	872.4	3.3
		T1		0.218	0.007	2.63	0.00					
romeo_27-72		S1		0.046	0.005	2.74	0.09	-5.27	-2.17	HRRIAHNKOJMXAS	920.3	3.6
		T1		0.070	0.009	2.51	0.06					
romeo_27-73		S1		0.049	0.003	2.79	0.05	-5.01	-1.92	FYCNLWFGCCPZBV	748.3	3.5
		T1		0.204	0.002	2.59	0.00					
romeo_27-74		S1		0.074	0.003	2.63	0.02	-4.82	-1.93	QQKHYWQZKKOIDM	816.3	3.1
		T1		0.018	0.001	2.42	0.02					

FIGURE 115

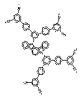
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_28-75		S1		0.068	0.005	2.68	0.04	-5.55	-2.19	VAUVLQCPXBQVOC	816.1	3.2
		T1		0.031	0.001	1.67	0.01					
romeo_29-76		S1		0.144	0.004	2.83	0.00	-5.12	-1.89	YMHVQJAKSXRKNU	980.3	3.6
		T1		0.194	0.003	2.63	0.00					
romeo_29-77		S1		0.087	0.004	2.78	0.01	-5.22	-1.94	BBLRDQLJXHURNH	676.2	3.4
		T1		0.092	0.005	2.51	0.01					
romeo_30-78		S1		0.040	0.010	2.83	0.22	-5.54	-2.35	YMPXYSHXQGAAMO	1216.4	4.2
		T1		0.096	0.006	2.63	0.02					
romeo_30-79		S1		0.038	0.003	2.61	0.07	-5.46	-2.29	TVMIQBTYLOPUQH	508.1	3.0
		T1		0.026	0.005	2.15	0.11					
romeo_31-82		S1		0.153	0.191	2.63	0.05	-5.09	-2.15	ZSRVLKUJJZNRPC	728.2	3.0
		T1		0.111	0.185	2.43	0.21					
romeo_31-83		S1		0.105	0.024	2.75	0.05	-5.02	-1.99	HDQWXOPLXKAVGG	880.2	3.2
		T1		0.141	0.024	2.58	0.01					
romeo_31-85		S1		0.009	0.004	2.72	0.24	-5.13	-2.11	JMLFRRWOXVSEPO	1132.3	4.3
		T1		0.142	0.004	2.54	0.00					

FIGURE 116

Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_32-86		S1		0.091	0.006	2.84	0.02	-4.71	-1.45	SFOZSTBUACYAJI	1020.4	3.4
		T1		0.214	0.004	2.63	0.00					
romeo_33-87		S1		0.117	0.008	2.79	0.01	-5.27	-2.11	AUNHZKNLIQDSDX	1024.4	3.7
		T1		0.123	0.011	2.56	0.01					
romeo_34-88		S1		0.138	0.003	2.82	0.00	-4.83	-1.63	UOGRFOKRBRFUIZ	762.3	2.8
		T1		0.205	0.003	2.62	0.00					
romeo_35-89		S1		0.039	0.003	2.62	0.06	-5.77	-2.74	SGANQHUROOAPSU	924.3	4.0
		T1		0.039	0.005	2.24	0.07					
romeo_36-91		S1		0.008	0.006	2.69	0.41	-4.75	-1.73	XHZCWOZJNDJFJQ	868.3	2.9
		T1		0.075	0.006	2.49	0.03					
romeo_36-92		S1		0.155	0.003	2.84	0.00	-5.09	-1.76	AJQBHNCBTBARGS	716.3	2.6
		T1		0.068	0.001	2.65	0.00					
romeo_37-93		S1		0.108	0.004	2.85	0.01	-4.95	-1.60	XSZCXVBJWMAJKX	676.2	3.3
		T1		0.199	0.002	2.64	0.00					
romeo_38-94		S1		0.043	0.010	2.66	0.17	-5.35	-2.32	FTZUEHWWWLKFGA	1048.2	4.0
		T1		0.034	0.011	2.32	0.22					

FIGURE 117

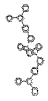
Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_38-95		S1		0.053	0.007	2.65	0.05	-4.96	-1.85	GOUPYBSCOYLFGA	744.1	3.9
		T1		0.071	0.010	2.43	0.06					
romeo_40-97		S1		0.169	0.203	2.77	0.03	-5.32	-2.18	GQECTFGBDFGLFB	968.1	3.4
		T1		0.154	0.197	2.55	0.06					
romeo_41-100		S1		0.027	0.003	2.74	0.10	-5.04	-1.98	SRDGHZUGEUCKSG	1022.4	3.3
		T1		0.040	0.003	2.55	0.06					
romeo_42-101		S1		0.033	0.005	2.80	0.16	-4.99	-1.82	ISBJXSKMASBENS	968.1	3.4
		T1		0.127	0.007	2.57	0.00					
romeo_43-102		S1		0.072	0.019	2.80	0.13	-5.00	-1.79	KQLUVXJXSRKGPS	924.4	3.2
		T1		0.203	0.017	2.59	0.00					
romeo_44-104		S1		0.099	0.011	2.86	0.04	-5.29	-2.01	IYKZMXFLQLPXCO	924.4	3.6
		T1		0.186	0.015	2.63	0.00					
romeo_44-105		S1		0.110	0.004	2.73	0.01	-5.77	-2.50	SLSOPHDBEWZBPH	508.1	2.8
		T1		0.083	0.002	2.36	0.01					
romeo_45-106		S1		0.114	0.004	2.84	0.01	-5.36	-2.01	TWFVPXYWLWNKDX	676.2	3.5
		T1		0.051	0.010	2.51	0.12					

FIGURE 118

Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_46-107		S1		0.060	0.004	2.89	0.05	-5.56	-2.23	UKBWFDRGZGSKBK	812.3	3.1
		T1		0.178	0.007	2.68	0.00					
romeo_47-108		S1		0.181	0.106	2.96	0.01	-5.48	-2.06	FJOXMRBFTPLONF	852.2	3.1
		T1		0.134	0.092	2.61	0.05					
romeo_49-110		S1		0.049	0.009	2.78	0.15	-5.36	-2.17	NXJRIHORJKCGBG	984.3	3.9
		T1		0.012	0.008	2.39	0.35					
romeo_50-111		S1		0.163	0.022	2.73	0.00	-4.96	-1.86	XMAJNXZQXDFUKV	776.2	3.1
		T1		0.100	0.005	2.51	0.01					
romeo_51-112		S1		0.220	0.092	2.65	0.00	-5.65	-2.50	IFSLABQXUDIDNZ	514.2	3.1
		T1		0.152	0.065	2.28	0.01					
romeo_51-113		S1		0.002	0.003	2.69	0.22	-5.15	-2.25	CYNBJIIXBAZFMY	874.4	3.6
		T1		0.123	0.003	2.52	0.00					
romeo_52-115		S1		0.033	0.004	2.80	0.12	-5.42	-2.22	NUQWWRVXCXQONC	920.3	3.6
		T1		0.134	0.005	2.57	0.00					
romeo_54-120		S1		0.031	0.009	2.74	0.28	-4.90	-1.90	PBNYKPMVJWUGCX	1022.4	3.2
		T1		0.143	0.010	2.56	0.00					

FIGURE 119

Name	Structure	Method	Color	Splitting (eV)	Strength	Absorp. (eV)	Rate (1/us)	HOMO (eV)	LUMO (eV)	INCHI Key	Weight	SA Score
romeo_54-121		S1		0.003	0.007	2.72	0.55	-4.85	-1.87	SFKBSWFCDLADTD	1106.5	3.7
		T1		0.002	0.007	2.53	0.47					
romeo_54-122		S1		0.103	0.006	2.83	0.01	-4.90	-1.80	ORJGURHESRBISR	1162.5	4.0
		T1		0.002	0.006	2.63	0.46					
romeo_54-123		S1		0.025	0.004	2.64	0.14	-4.93	-1.98	KAEKOCIESRMFCC	1022.4	3.2
		T1		0.023	0.005	2.41	0.14					
romeo_54-124		S1		0.003	0.003	2.66	0.22	-4.81	-1.90	RLWBLXVQXGFEFL	1078.5	3.5
		T1		0.064	0.003	2.47	0.02					

FIGURE 120

ORGANIC LIGHT-EMITTING DIODE MATERIALS

RELATED APPLICATIONS

[0001] This application claims the benefit of U.S. Provisional Application No. 62/191766, filed on Jul. 13, 2015; U.S. Provisional Application No. 62/208190, filed on Aug. 21, 2015; U.S. Provisional Application No. 62/239556, filed on Oct. 9, 2015; U.S. Provisional Application No. 62/277316, filed on Jan. 11, 2016. The entire teachings of each application above are incorporated herein by reference.

BACKGROUND OF THE INVENTION

[0002] An organic light emitting diode (OLED) is a light-emitting diode (LED) in which a film of organic compounds is placed between two conductors and emits light in response to excitation, such as an electric current. OLEDs are useful in displays such as television screen, computer monitors, mobile phones, and tablets. A problem inherent in OLED displays is the limited lifetime of the organic materials. OLEDs which emit blue light, in particular, degrade at a significantly increased rate as compared to green or red OLEDs.

[0003] OLED materials rely on the radiative decay of molecular excited states (excitons) generated by recombination of electrons and holes in a host transport material. The nature of excitation results in interactions between electrons and holes that split the excited states into bright singlets (with a total spin of 0) and dark triplets (with a total spin of 1). Since the recombination of electrons and holes affords a statistical mixture of four spin states (one singlet and three triplet sublevels), conventional OLEDs have a maximum theoretical efficiency of 25%.

[0004] To date, OLED material design has focused on harvesting the remaining energy from the normally dark triplets into an emissive state. Recent work to create efficient phosphors, which emit light from the normally dark triplet state, have resulted in green and red OLEDs. Other colors, such as blue, however, require higher energy excited states which enhance the degradation process of the OLED.

[0005] The fundamental limiting factor to the triplet-singlet transition rate is a value of the parameter $|H_{fi}/\Delta|^2$, where H_{fi}, is the coupling energy due to hyperfine or spin-orbit interactions, and Δ is the energetic splitting between singlet and triplet states. Traditional phosphorescent OLEDs rely on the mixing of singlet and triplet states due to spin-orbital (SO) interaction, increasing H_{fi} and affording a lowest emissive state shared between a heavy metal atom and an organic ligand. This results in energy harvesting from all higher singlet and triplet states, followed by phosphorescence (relatively short-lived emission from the excited triplet). The shortened triplet lifetime reduces triplet exciton annihilation by charges and other excitons. Recent work by others suggests that the limit to the performance of phosphorescent materials has been reached.

SUMMARY OF THE INVENTION

[0006] Thus, a need exists for OLEDs which can reach higher excitation states without rapid degradation. It has now been discovered that thermally activated delayed fluorescence (TADF), which relies on minimization of Δ as opposed to maximization of H_{fi}, can transfer population between singlet levels and triplet sublevels in a relevant timescale, such as, for example, 110 μs. The compounds described herein are capable of fluorescing or phosphorescing at higher energy excitation states than compounds previously described.

[0007] Accordingly, in one embodiment, the present invention is a molecule represented by one of structural formulas (I), (II), (IIIA)-(IIIE), (IIIC), (IV), (VA)-(VL), (VI), (VIIA)-(VIIE), or (VIIIA)-(VIIIF).

[0008] In another embodiment, the present invention is a molecule represented by one of the structural formulas in Tables M, N, O, Q, B, or R.

[0009] In another embodiment, the present invention is an organic light-emitting device comprising a first electrode, a second electrode, and an organic layer between the first electrode and the second electrode. The organic layer comprises at least one light-emitting molecule selected from the compounds disclosed herein.

BRIEF DESCRIPTION OF THE DRAWINGS

[0010] The foregoing will be apparent from the following more particular description of example embodiments of the invention, as illustrated in the accompanying drawings in which like reference characters refer to the same parts throughout the different views. The drawings are not necessarily to scale, emphasis instead being placed upon illustrating embodiments of the present invention.

[0011] FIGS. **1-21** represent Table 1 which lists example embodiments of the present invention.

[0012] FIGS. **22** to **40** represent Table 2 which lists example embodiments of the present invention.

[0013] FIGS. **41** to **48** represent Table 3 which lists example embodiments of the present invention.

[0014] FIGS. **49** to **57** represent Table 4 which lists example embodiments of the present invention.

[0015] FIGS. **58** to **72** represent Table 5 which lists example embodiments of the present invention.

[0016] FIGS. **73** to **89** represent Table 6 which lists example embodiments of the present invention.

[0017] FIGS. **90** to **91** represent Table 7 which lists example embodiments of the present invention.

[0018] FIGS. **92** to **93** represent Table 8 which lists example embodiments of the present invention.

[0019] FIGS. **94** to **98** represent Table 9 which lists example embodiments of the present invention.

[0020] FIGS. **99-104** represent Table 10, which lists example embodiments of the present invention.

[0021] FIGS. **105-107** represent Table 11, which lists example structures.

[0022] FIGS. **108-120** represent Table 12, which lists example embodiments of the present invention.

DETAILED DESCRIPTION OF THE INVENTION

[0023] A description of example embodiments of the invention follows.

Glossary

[0024] The term "alkyl," as used herein, refers to a saturated aliphatic branched or straight-chain monovalent hydrocarbon radical having the specified number of carbon atoms. Thus, "C_1-C_6 alkyl" means a radical having from 1-6 carbon atoms in a linear or branched arrangement. Examples of "C_1-C_6 alkyl" include, n-propyl, i-propyl, n-butyl, i-butyl,

sec-butyl, t-butyl, n-pentyl, n-hexyl, 2-methylbutyl, 2-methylpentyl, 2-ethylbutyl, 3-methylpentyl, and 4-methylpentyl. An alkyl can be optionally substituted with halogen, —OH, C_1-C_6 alkyl, C_1-C_6 alkoxy, —NO_2, —CN, and —$N(R^1)(R^2)$ wherein R^1 and R^2 are each independently selected from —H and C_1-C_3 alkyl.

[0025] The term "alkenyl," as used herein, refers to a straight-chain or branched alkyl group having one or more carbon-carbon double bonds. Thus, "C_2-C_6 alkenyl" means a radical having 2-6 carbon atoms in a linear or branched arrangement having one or more double bonds. Examples of "C_2-C_6 alkenyl" include ethenyl, propenyl, butenyl, pentenyl, hexenyl, butadienyl, pentadienyl, and hexadienyl. An alkenyl can be optionally substituted with the substituents listed above with respect to alkyl.

[0026] The term "alkynyl," as used herein, refers to a straight-chain or branched alkyl group having one or more carbon-carbon triple bonds. Thus, "C_2-C_6 alkynyl" means a radical having 2-6 carbon atoms in a linear or branched arrangement having one or more triple bonds. Examples of C_2-C_6 "alkynyl" include ethynyl, propynyl, butynyl, pentynyl, and hexynyl. An alkynyl can be optionally substituted with the substituents listed above with respect to alkyl.

[0027] The term "cycloalkyl," as used herein, refers to a saturated monocyclic or fused polycyclic ring system containing from 3-12 carbon ring atoms. Saturated monocyclic cycloalkyl rings include, for example, cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, and cyclooctyl. Saturated bicyclic and polycyclic cycloalkyl rings include, for example, norbornane, [2.2.2]bicyclooctane, decahydronaphthalene and adamantane. A cycloalkyl can be optionally substituted with the substituents listed above with respect to alkyl.

[0028] The term "amino," as used herein, means an "—NH_2," an "NHR_p," or an "NR_pR_q," group, wherein R_p and R_q can be alkyl, alkenyl, alkynyl, alkoxy, cycloalkyl, aryl, and heteroaryl. Amino may be primary (NH_2), secondary (NHR_p) or tertiary (NR_pR_q).

[0029] The term "alkylamino," as used herein, refers to an "NHR_p," or an "NR_pR_q" group, wherein R_p and R_q can be alkyl, alkenyl, alkynyl, alkoxy, or cycloalkyl. The term "dialkylamino," as used herein, refers to an "NR_pR_q" group, wherein R_p and R_q can be alkyl, alkenyl, alkynyl, alkoxy, or cycloalkyl.

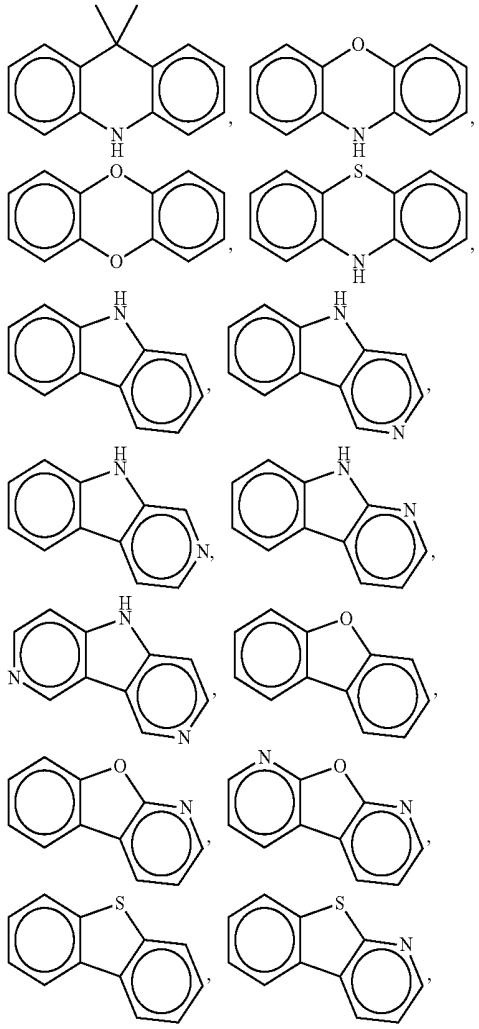
[0030] The term "alkoxy", as used herein, refers to an "alkyl-O" group, wherein alkyl is defined above. Examples of alkoxy group include methoxy or ethoxy groups. The "alkyl" portion of alkoxy can be optionally substituted as described above with respect to alkyl.

[0031] The term "aryl," as used herein, refers to an aromatic monocyclic or polycyclic ring system consisting of carbon atoms. Thus, "C_6-C_{18} aryl" is a monocylic or polycyclic ring system containing from 6 to 18 carbon atoms. Examples of aryl groups include phenyl, indenyl, naphthyl, azulenyl, heptalenyl, biphenyl, indacenyl, acenaphthylenyl, fluorenyl, phenalenyl, phenanthrenyl, anthracenyl, cyclopentacyclooctenyl or benzocyclooctenyl. An aryl can be optionally substituted with halogen, —OH, C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, C_1-C_6 haloalkyl, C_1-C_6 alkoxy, C_6-C_{18} aryl, C_6-C_{18} haloaryl, (5-20 atom) heteroaryl, —$C(O)C_1$-C_3 haloalkyl, —$S(O)_2$—, —NO_2, —CN, and oxo.

[0032] The terms "halogen," or "halo," as used herein, refer to fluorine, chlorine, bromine, or iodine.

[0033] The term "heteroaryl," as used herein, refers a monocyclic or fused polycyclic aromatic ring containing one or more heteroatoms, such as oxygen, nitrogen, or sulfur. For example, a heteroaryl can be a "5-20 atom heteroaryl," which means a 5 to 20 membered monocyclic or fused polycyclic aromatic ring containing at least one heteroatom. Examples of heteroaryl groups include pyridinyl, pyridazinyl, imidazolyl, pyrimidinyl, pyrazolyl, triazolyl, pyrazinyl, quinolyl, isoquinolyl, tetrazolyl, furyl, thienyl, isoxazolyl, thiazolyl, oxazolyl, isothiazolyl, pyrrolyl, quinolinyl, isoquinolinyl, indolyl, benzimidazolyl, benzofuranyl, cinnolinyl, indazolyl, indolizinyl, phthalazinyl, pyridazinyl, triazinyl, isoindolyl, purinyl, oxadiazolyl, thiazolyl, thiadiazolyl, furazanyl, benzofurazanyl, benzothiophenyl, benzotriazolyl, benzothiazolyl, benzoxazolyl, quinazolinyl, quinoxalinyl, naphthyridinyl, dihydroquinolyl, tetrahydroquinolyl, dihydroisoquinolyl, tetrahydroisoquinolyl, benzofuryl, furopyridinyl, pyrolopyrimidinyl, and azaindolyl. A heteroaryl can be optionally substituted with the same substituents listed above with respect to aryl.

[0034] In other embodiments, a "5-20 member heteroaryl" refers to a fused polycyclic ring system wherein aromatic rings are fused to a heterocycle. Examples of these heteroaryls include:



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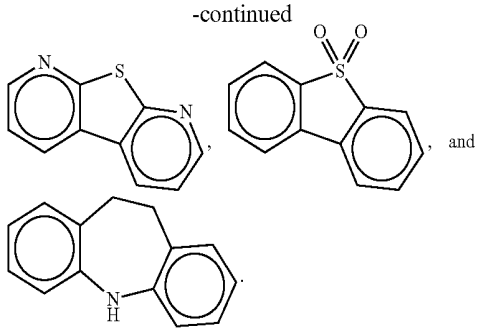


[0035] The term "haloalkyl," as used herein, includes an alkyl substituted with one or more of F, Cl, Br, or I, wherein alkyl is defined above. The "alkyl" portion of haloalkyl can be optionally substituted as described above with respect to alkyl.

[0036] The term "haloaryl," as used herein, includes an aryl substituted with one or more of F, Cl, Br, or I, wherein aryl is defined above. The "aryl" portion of haloaryl can be optionally substituted as described above with respect to aryl.

[0037] The term "oxo," as used herein, refers to =O.

[0038] The term "nitro," as used herein, refers to —NO_2.

[0039] The term "symmetrical molecule," as used herein, refers to molecules that are group symmetric or synthetic symmetric. The term "group symmetric," as used herein, refers to molecules that have symmetry according to the group theory of molecular symmetry. The term "synthetic symmetric," as used herein, refers to molecules that are selected such that no regioselective synthetic strategy is required.

[0040] The term "donor," as used herein, refers to a molecular fragment that can be used in organic light emitting diodes and is likely to donate electrons from its highest occupied molecular orbital to an acceptor upon excitation. In an example embodiment, donors have an ionization potential greater than or equal to −6.5 eV.

[0041] The term "acceptor," as used herein, refers to a molecular fragment that can be used in organic light emitting diodes and is likely to accept electrons into its lowest unoccupied molecular orbital from a donor that has been subject to excitation. In an example embodiment, acceptors have an electron affinity less than or equal to −0.5 eV.

[0042] The term "bridge," as used herein, refers to π-conjugated molecular fragment that can be included in a molecule which is covalently linked between acceptor and donor moieties. The bridge can, for example, be further conjugated to the acceptor moiety, the donor moiety, or both. Without being bound to any particular theory, it is believed that the bridge moiety can sterically restrict the acceptor and donor moieties into a specific configuration, thereby preventing the overlap between the conjugated π system of donor and acceptor moieties. Examples of suitable bridge moieties include phenyl, ethenyl, and ethynyl.

[0043] The term "multivalent," as used herein, refers to a molecular fragment that is connected to at least two other molecular fragments. For example, a bridge moiety, is multivalent.

[0044] "〰" as used herein, refers to a point of attachment between two atoms.

Principles of OLED

[0045] OLEDs are typically composed of a layer of organic materials or compounds between two electrodes, an anode and a cathode. The organic molecules are electrically conductive as a result of delocalization of π C electronics caused by conjugation over part or all of the molecule. When voltage is applied, electrons from the highest occupied molecular orbital (HOMO) present at the anode flow into the lowest unoccupied molecular orbital (LUMO) of the organic molecules present at the cathode. Removal of electrons from the HOMO is also referred to as inserting electron holes into the HOMO. Electrostatic forces bring the electrons and the holes towards each other until they recombine and form an exciton (which is the bound state of the electron and the hole). As the excited state decays and the energy levels of the electrons relax, radiation is emitted having a frequency in the visible spectrum. The frequency of this radiation depends on the band gap of the material, which is the difference in energy between the HOMO and the LUMO.

[0046] As electrons and holes are fermions with half integer spin, an exciton may either be in a singlet state or a triplet state depending on how the spins of the electron and hole have been combined. Statistically, three triplet excitons will be formed for each singlet exciton. Decay from triplet states is spin forbidden, which results in increases in the timescale of the transition and limits the internal efficiency of fluorescent devices. Phosphorescent organic light-emitting diodes make use of spin-orbit interactions to facilitate intersystem crossing between singlet and triplet states, thus obtaining emission from both singlet and triplet states and improving the internal efficiency.

[0047] The prototypical phosphorescent material is iridium tris(2-phenylpyridine) ($Ir(ppy)_3$) in which the excited state is a charge transfer from the Ir atom to the organic ligand. Such approaches have reduced the triplet lifetime to about 1 μs, several orders of magnitude slower than the radiative lifetimes of fully-allowed transitions such as fluorescence. Ir-based phosphors have proven to be acceptable for many display applications, but losses due to large triplet densities still prevent the application of OLEDs to solid-state lighting at higher brightness.

[0048] Further, recent research suggests that traditional Iridium based OLEDs may have reached a physical performance limit. As illustrated in FIG. **1**, the brightness of an OLED will decrease as the time of decay increases. Since the highest energy triplet state is the origin of the luminescent transition in the Ir-based materials of FIG. **1**, increasing the zero-field splitting through additional spin-orbit coupling will eventually lengthen the effective lifetime of the other two triplets. It is believed that this effect is responsible for the asymptote empirically observed at about 1 μs.

[0049] The recently developed thermally activated delayed fluorescence (TADF) seeks to minimize energetic splitting between singlet and triplet states (Δ). The reduction in exchange splitting from typical values of 0.4-0.7 eV to a gap of the order of the thermal energy (proportional to k_BT, where k_B represents the Boltzmann constant, and T represents temperature) means that thermal agitation can transfer population between singlet levels and triplet sublevels in a relevant timescale even if the coupling between states is small.

[0050] Example TADF molecules consist of donor and acceptor moieties connected directly by a covalent bond or via a conjugated linker (or "bridge"). A "donor" moiety is

likely to transfer electrons from its HOMO upon excitation to the "acceptor" moiety. An "acceptor" moiety is likely to accept the electrons from the "donor" moiety into its LUMO. The donor-acceptor nature of TADF molecules results in low-lying excited states with charge-transfer character that exhibit very low Δ. Since thermal molecular motions can randomly vary the optical properties of donor-acceptor systems, a rigid three-dimensional arrangement of donor and acceptor moieties can be used to limit the non-radiative decay of the charge-transfer state by internal conversion during the lifetime of the excitation.

[0051] It is beneficial, therefore, to decrease energetic splitting between singlet and triplet states (Δ), and to create a system with increased reversed intersystem crossing (RISC) capable of exploiting triplet excitons. Such a system, it is believed, will result in decreased emission lifetimes. Systems with these features will be capable of emitting blue light without being subject to the rapid degradation prevalent in blue OLEDs known today.

Compounds of the Invention

[0052] The molecules of the present invention, when excited via thermal or electronic means, can produce light in the blue or green region of the visible spectrum. The molecules comprise molecular fragments including at least one donor moiety, at least one acceptor moiety, and optionally, a bridge moiety.

[0053] Electronic properties of the example molecules of the present invention can be computed using known ab initio quantum mechanical computations. By scanning a library of small chemical compounds for specific quantum properties, molecules can be constructed which exhibit the desired spin-orbit/thermally activated delayed fluorescence (SO/TADF) properties described above.

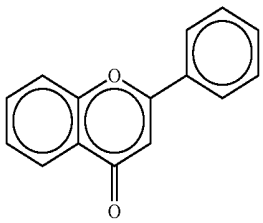
[0054] It could be beneficial, for example, to build molecules of the present invention using molecular fragments with a calculated triplet state above 2.75 eV. Therefore, using a time-dependent density functional theory using, as a basis set, the set of functions known as 6-31G* and a Becke, 3-parameter, Lee-Yang-Parr hybrid functional to solve Hartree-Fock equations (TD-DFT/B3LYP/6-31G*), molecular fragments (moieties) can be screened which have HOMOs above a specific threshold and LUMOs below a specific threshold, and wherein the calculated triplet state of the moieties is above 2.75 eV.

[0055] Therefore, for example, a donor moiety ("D") can be selected because it has a HOMO energy (e.g., an ionization potential) of greater than or equal to −6.5 eV. An acceptor moiety ("A") can be selected because it has, for example, a LUMO energy (e.g., an electron affinity) of less than or equal to −0.5 eV. The bridge moiety ("B") can be a rigid conjugated system which can, for example, sterically restrict the acceptor and donor moieties into a specific configuration, thereby preventing the overlap between the conjugated π system of donor and acceptor moieties.

[0056] Accordingly, in a first aspect, the present invention is a molecule comprising at least one acceptor moiety A, at least one donor moiety D, and optionally, a bridge moiety B. The moiety D, for each occurrence independently, is a monocyclic or fused polycyclic aryl or heteroaryl having between 5 and 20 atoms, optionally substituted with one or more substituents. The moiety A, for each occurrence independently, is —CF_3, —CN, or a monocyclic or fused polycyclic aryl or heteroaryl having between 5 and 20 atoms, optionally substituted with one or more substituents. The moiety B, for each occurrence independently, is phenyl optionally substituted with one to four substituents. Each moiety A is covalently attached to either the moiety B or the moiety D, each moiety D is covalently attached to either the moiety B or the moiety A, and each moiety B is covalently attached to at least one moiety A and at least one moiety D. At least one moiety A is selected from list AN1 or at least one moiety D is selected from list DN1.

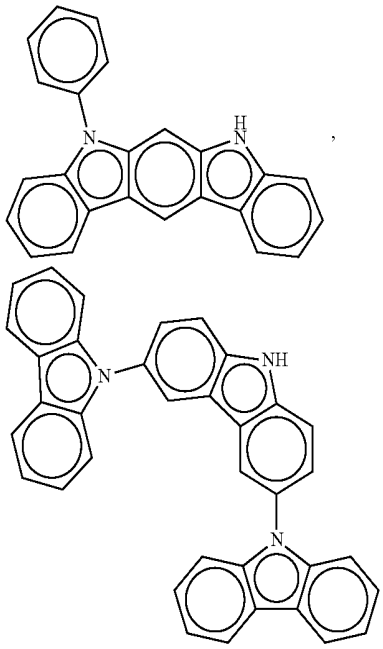
List AN1

[0057]



List DN1

[0058]



In an example embodiment of the first aspect, each moiety A is bonded either to moiety B or moiety D, each moiety B is bonded either to moiety A, moiety D, or a second moiety B, and each moiety D is bonded either to moiety A or moiety B. In another example embodiment of the first aspect, the moieties A are different than the moieties D.

[0059] The foregoing rules of connection mean that the moiety A cannot be connected to another moiety A, the moiety D cannot be connected to another moiety D, and that each moiety B is multivalent, and therefore must be connected to at least two other moieties, either a moiety A, a

moiety D, or a second moiety B. It is understood that within a molecule no molecular fragment represented by A is the same as any molecular fragment represented by D.

[0060] In a second aspect, the present invention is a molecule comprising at least one acceptor moiety A, at least one donor moiety D, and optionally, one or more bridge moieties B; wherein A, D, and B are defined above with respect to the first aspect of the present invention, and wherein at least one moiety A is selected from list AN1 or at least one moiety D is selected from list DN1. In addition to the moieties recited above in the first aspect, the moiety D can be —$N(C_6$-C_{18}aryl$)_2$. In addition to the moieties recited above with respect to the first aspect, the moiety A, can be —$S(O)_2$—. In addition to the moieties recited above with respect to the first aspect, the moiety B can be C_2-C_6 alkenyl, C_2-C_6 alkynyl, or C_5-C_{12} cycloalkyl optionally substituted with one to four substituents.

[0061] In a third aspect, the present invention is a molecule defined by the structural formula (G-I)

$$(A)_m\text{-}(B)_l\text{-}(D)_p \quad \text{(G-I)}$$

[0062] wherein A, B, and D are defined above with respect to the first and second aspects, at least one moiety A is selected from list AN1, and at least one moiety D is selected from list DN1, and

[0063] the moiety D, for each occurrence independently, is optionally substituted with one or more substituents each independently selected from C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, C_6-C_{18} aryl, (5-20 atom) heteroaryl, C_1-C_6 alkoxy, amino, C_1-C_3 alkylamino, C_1-C_3 dialkylamino, or oxo;

[0064] the moiety A, for each occurrence independently, is optionally substituted with one or more substituents independently selected from C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, C_6-C_{18} aryl, (5-20 atom) heteroaryl, C_1-C_6 alkoxy, —$C(O)C_1$-C_3 haloalkyl, —$S(O_2)H$, —NO_2, —CN, oxo, halogen, or C_6-C_{18} haloaryl;

[0065] the moiety B, for each occurrence independently, is optionally substituted with one to four substituents, each independently selected from C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, C_6-C_{18} aryl, or (5-20 atom) heteroaryl;

[0066] m is an integer greater than 1;

[0067] p is an integer greater than 1; and

[0068] l is either 0 or an integer greater than one. In an example embodiment, l is greater than 1. In another example embodiment, 1 is 0, 1, or 2.

[0069] In a fourth aspect, the present invention is a molecule defined by the structural formula (G-I)

$$(A)_m\text{-}(B)_l\text{-}(D)_p \quad \text{(G-I)}$$

[0070] wherein A, B, and D are defined above with respect to the first or second aspects of the present invention, at least one moiety A is selected from list AN1, and at least one moiety D is selected from list DN1, and

[0071] the moiety D, for each occurrence independently, is optionally substituted, in addition to the substituents described above with respect to the third aspect of the present invention, with —$N(C_6$-C_{18} aryl$)_2$;

[0072] the moiety A, for each occurrence independently, is optionally substituted as described above with respect to the third aspect of the present invention;

[0073] the moiety B, for each occurrence independently, is optionally substituted as described above with respect to the third aspect of the present invention;

[0074] m is an integer greater than 1;

[0075] p is an integer greater than 1; and

[0076] l is either 0 or an integer greater than one. In an example embodiment, l is greater than 1. In another example embodiment, 1 is 0, 1, or 2.

[0077] In a fifth aspect, the present invention is molecule defined by the structural formula (G-I)

$$(A)_m\text{-}(B)_l\text{-}(D)_p \quad \text{(G-I)}$$

[0078] wherein A, B, and D are defined above with respect to the first and second aspects of the present invention, at least one moiety A is selected from list AN1, and at least one moiety D is selected from list DN1, and

[0079] the moiety D, for each occurrence independently, is optionally substituted as described above with respect to the third and fourth aspects, and further wherein, each alkyl, alkenyl, alkynyl, aryl, and heteroaryl optionally further substituted with one or more substituents selected from C_1-C_6 alkyl, 5-20 atom heteroaryl, or —$N(C_6$-C_{18}aryl$)_2$;

[0080] the moiety A, for each occurrence independently, is optionally substituted as described above with respect to the third aspect of the present invention;

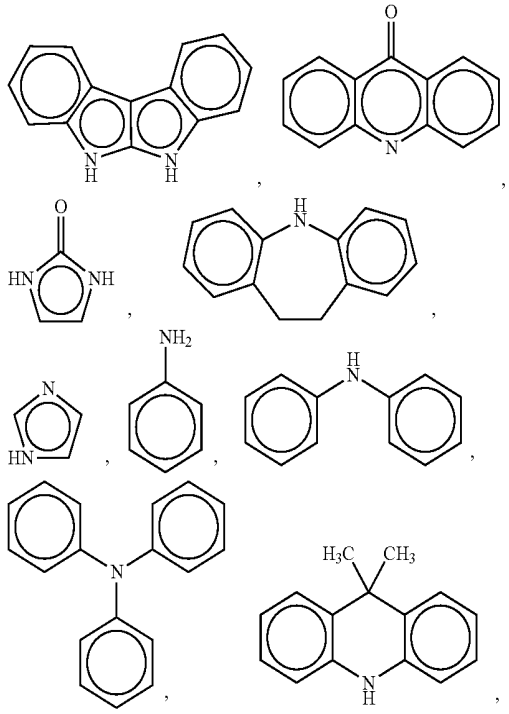
[0081] the moiety B, for each occurrence independently, is optionally substituted as described above with respect to the third aspect of the present invention;

[0082] m is an integer greater than 1;

[0083] p is an integer greater than 1; and

[0084] l is either 0 or an integer greater than one. In an example embodiment, l is greater than 1. In another example embodiment, 1 is 0, 1, or 2.

[0085] In a sixth aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety D, for each occurrence independently, can be selected from List D1.



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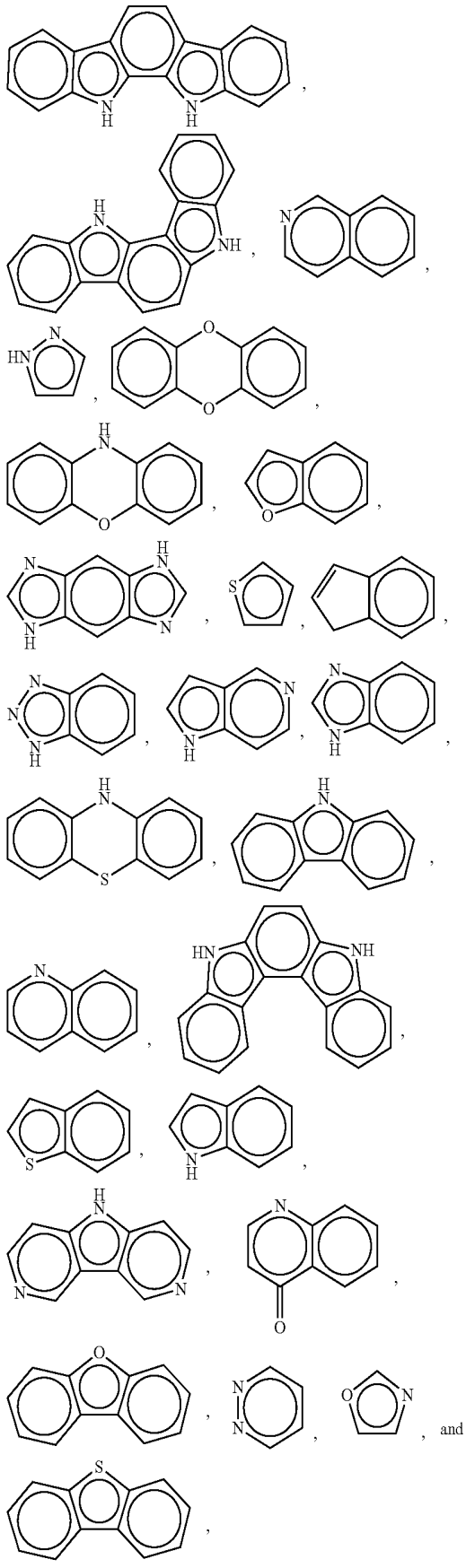
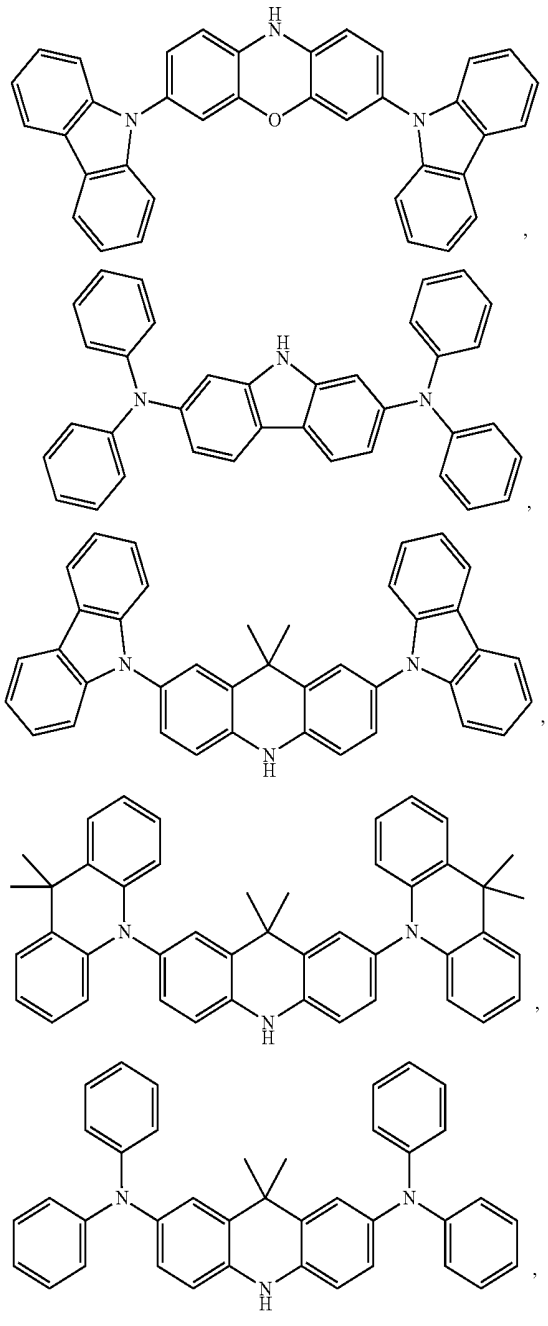


and wherein the moiety D can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0086] In a seventh aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety D, for each occurrence independently, can be selected from List D1, List D2, or both.

List D2

[0087]



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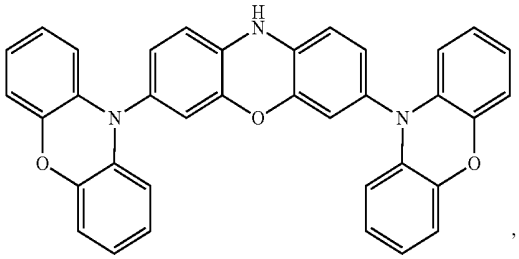

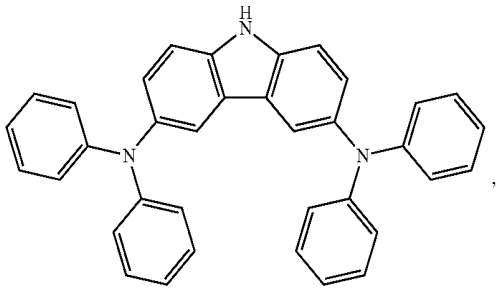

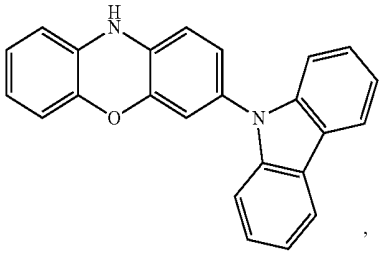

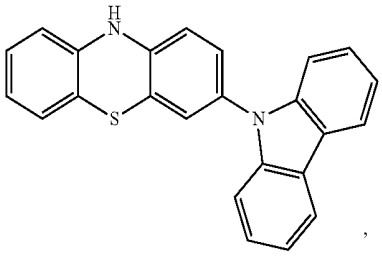

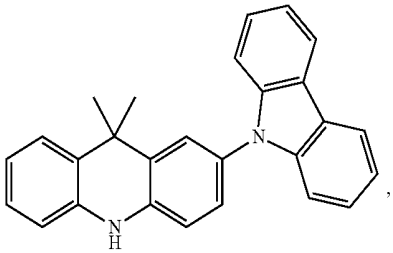

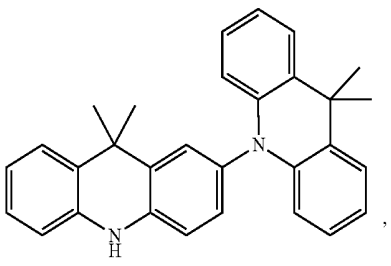

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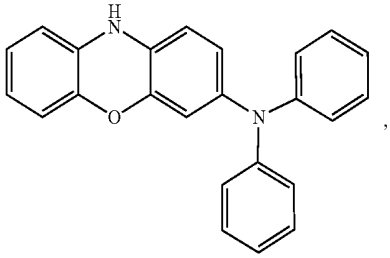

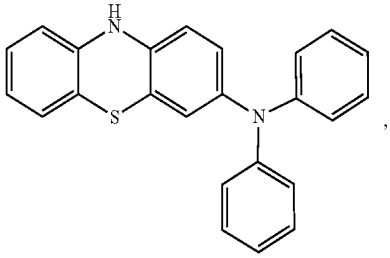

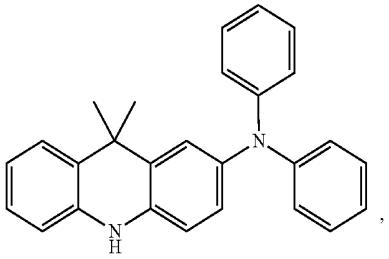

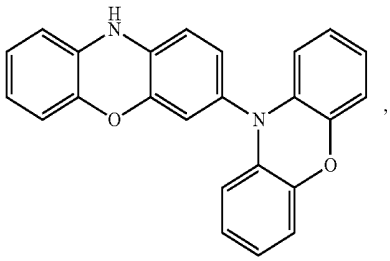

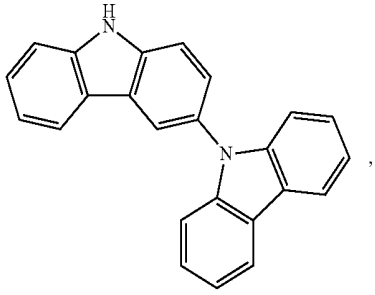

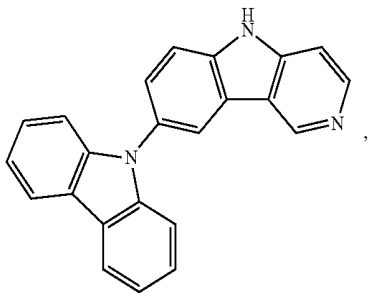

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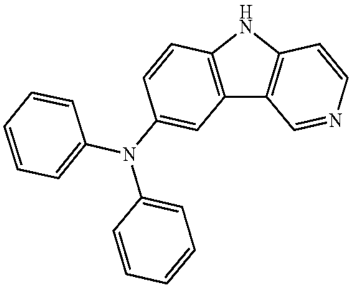
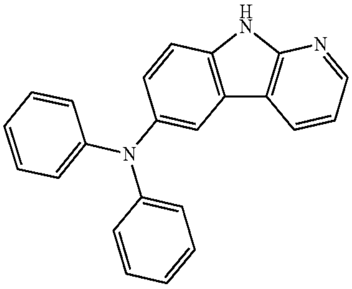
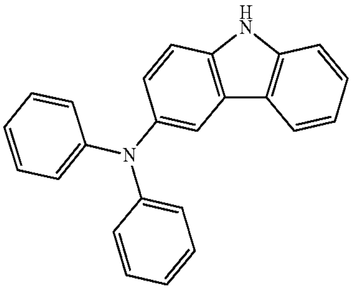
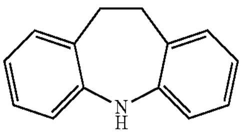
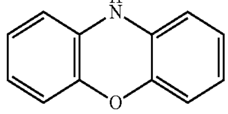
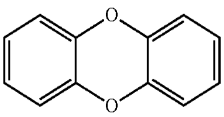
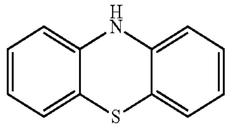
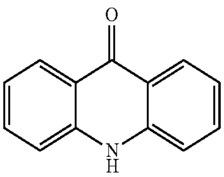
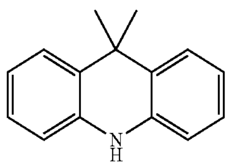
 ,

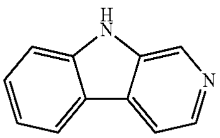
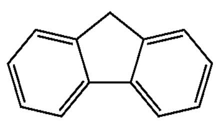
 ,

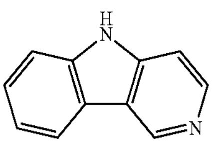
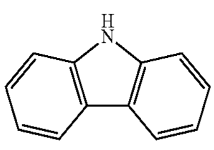
 ,

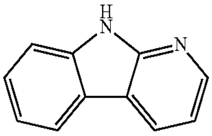
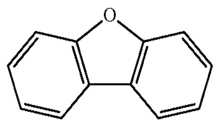
 ,  ,

 ,  ,

 ,  ,

 ,  ,

 ,  ,

 ,  ,

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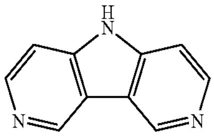
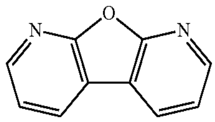
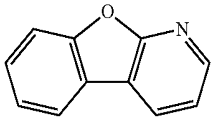
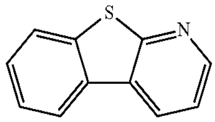
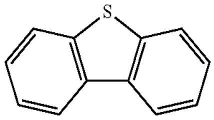
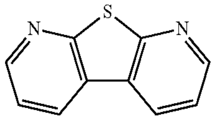
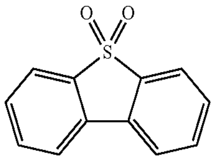
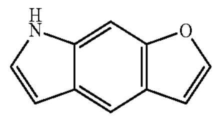
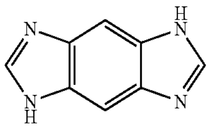
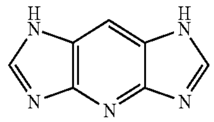
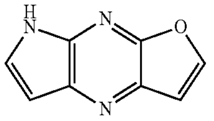
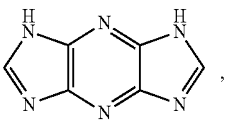
 ,  ,

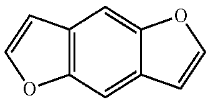
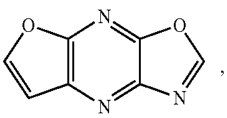
 ,  ,

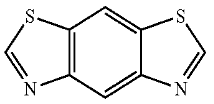
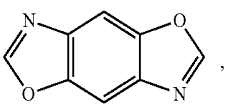
 ,  ,

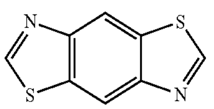
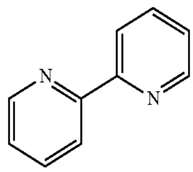
 ,  ,

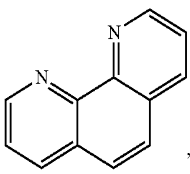
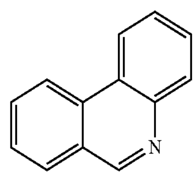
 ,  ,

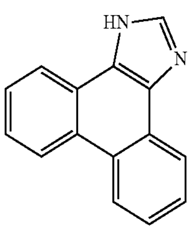
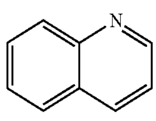
 ,  ,

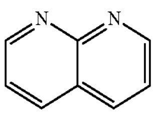
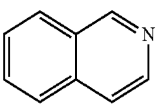
 ,  ,

 ,  ,

 ,  ,

 ,  ,

 ,  ,

 ,  ,

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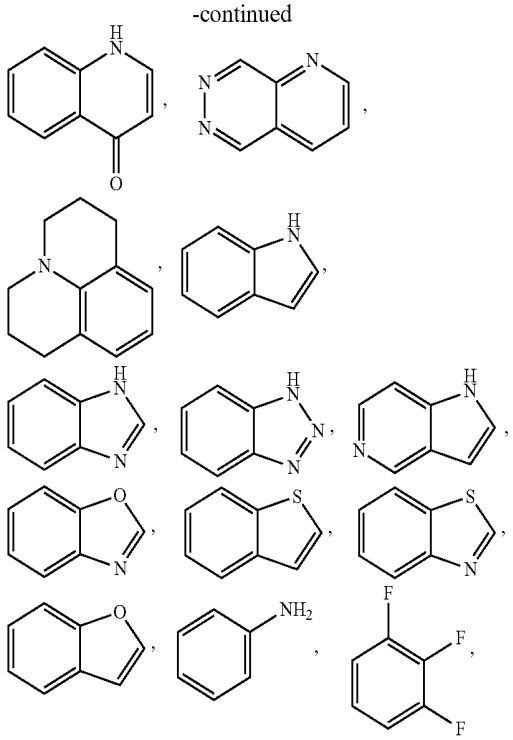

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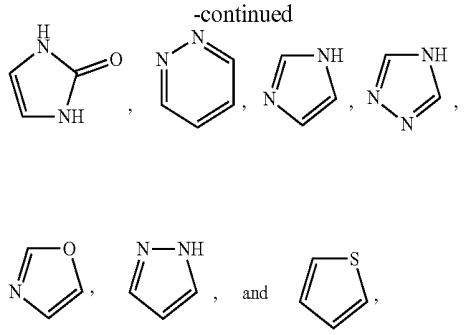
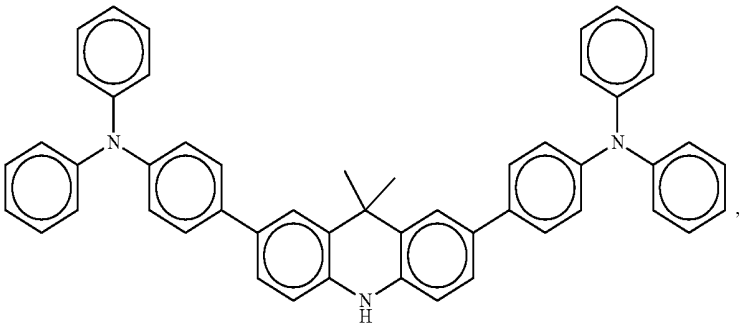


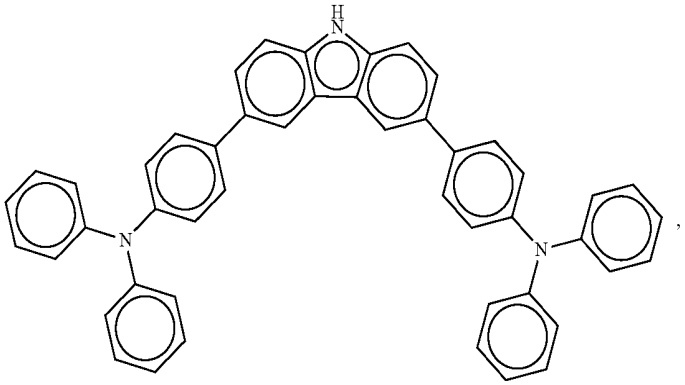
and wherein the moiety D can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0088] In a eighth aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety D, for each occurrence independently, can be selected from List D1, List D2, List D3, or any combination thereof.

List D3

[0089]





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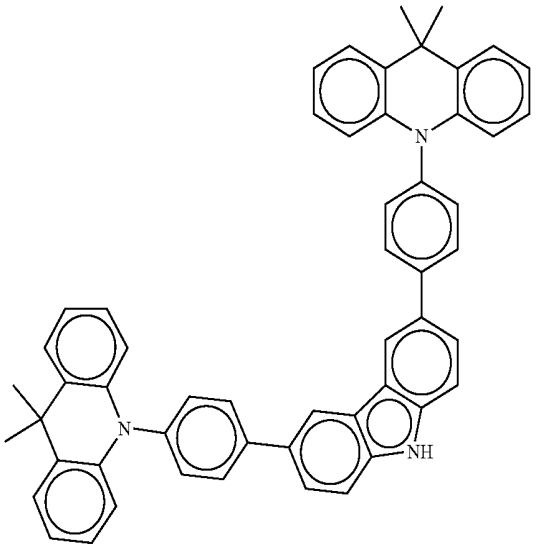

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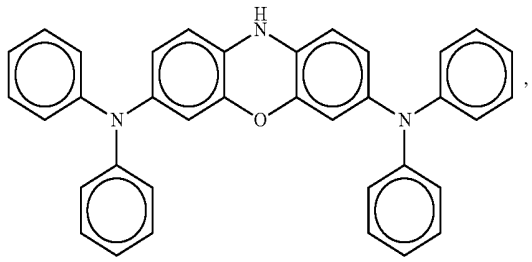

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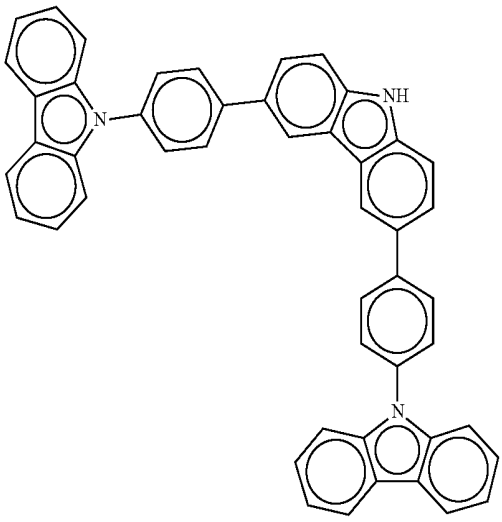

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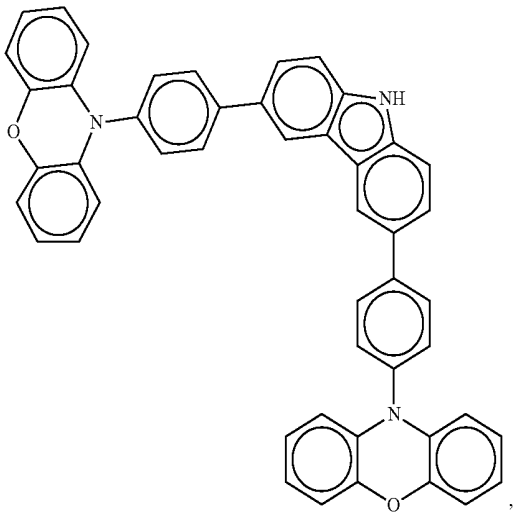

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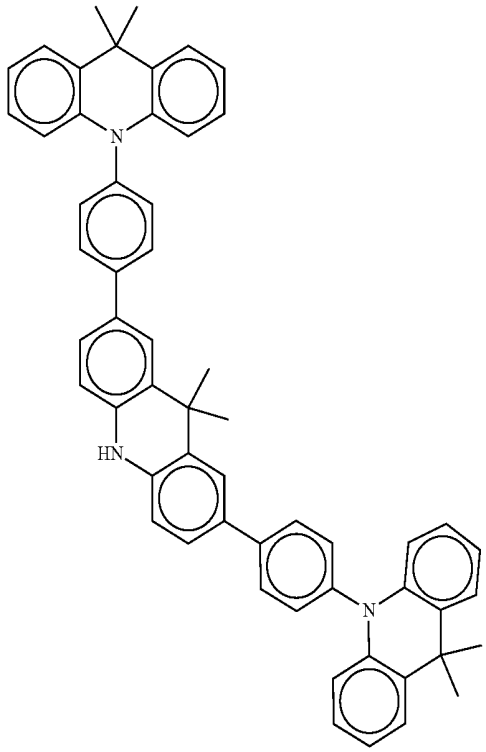

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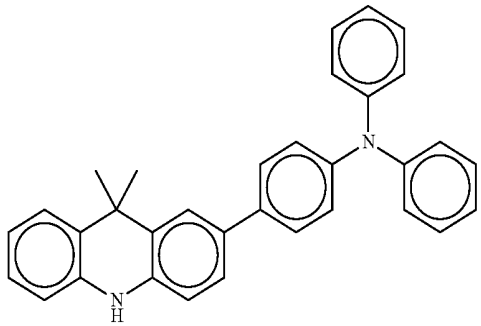

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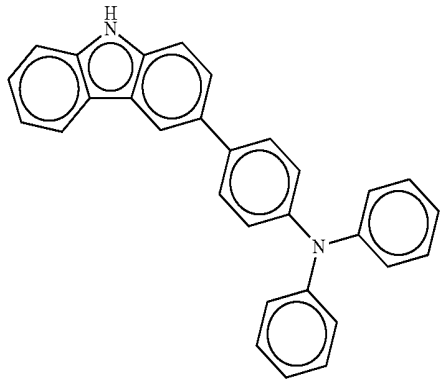

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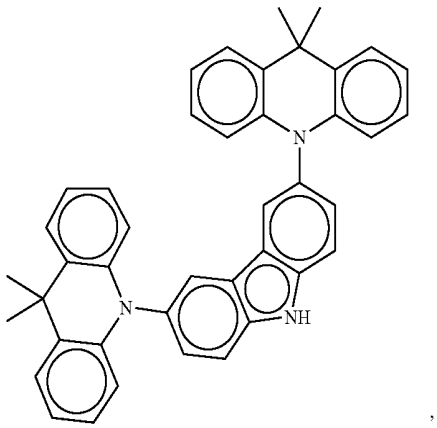

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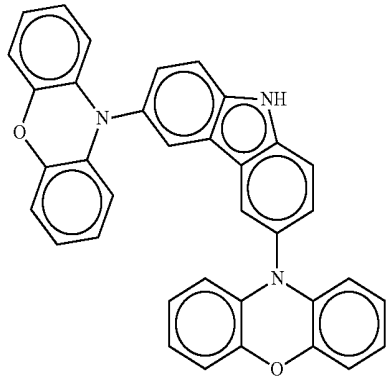

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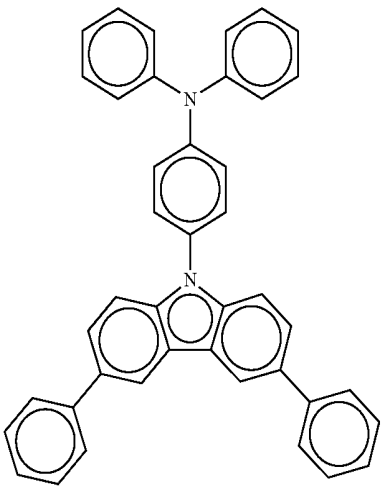

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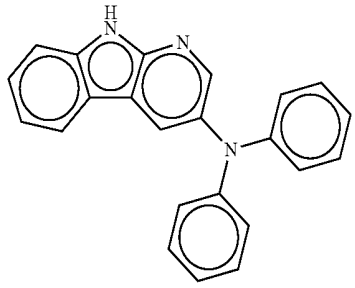
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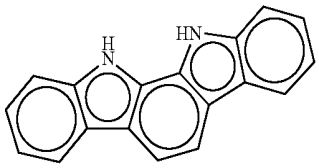
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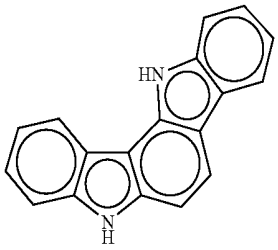
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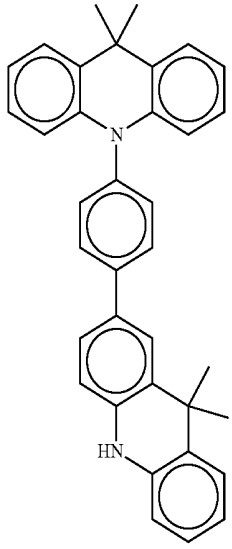
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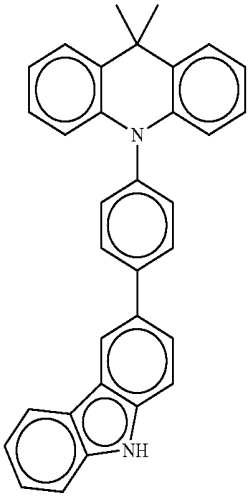
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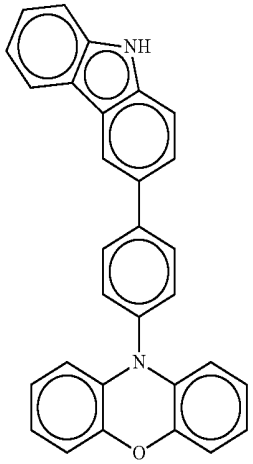
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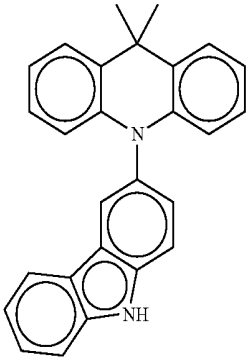
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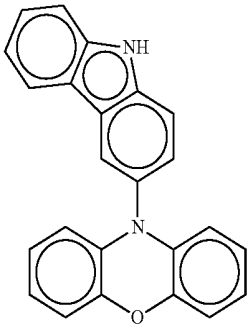
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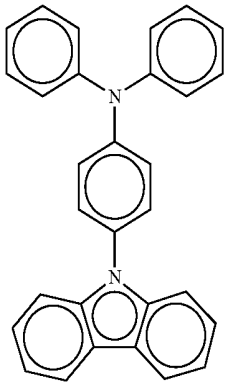
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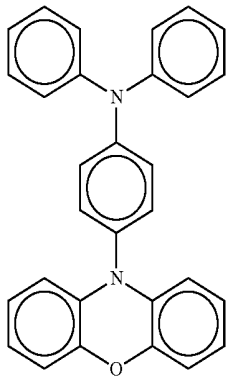
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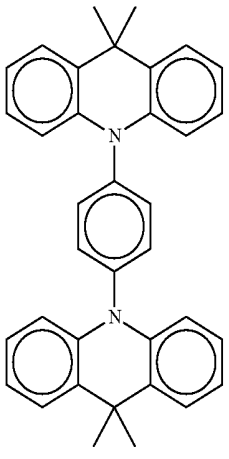
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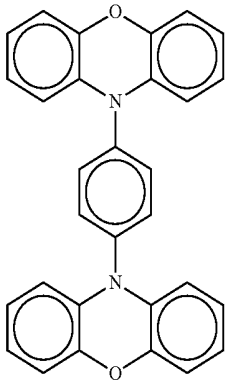
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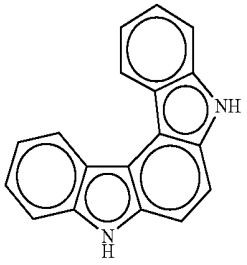
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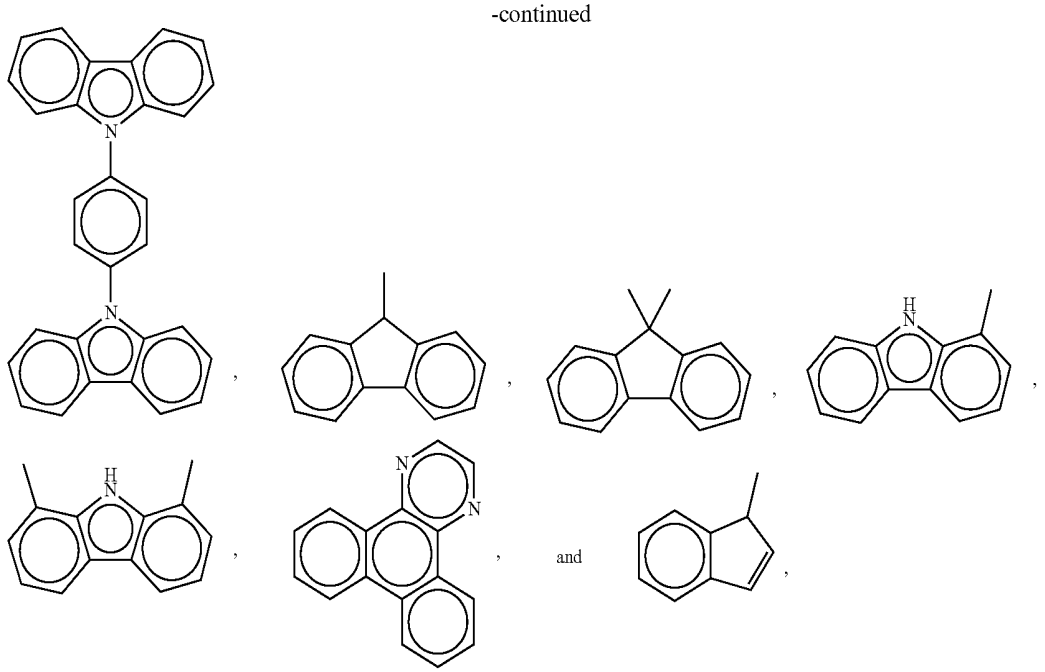
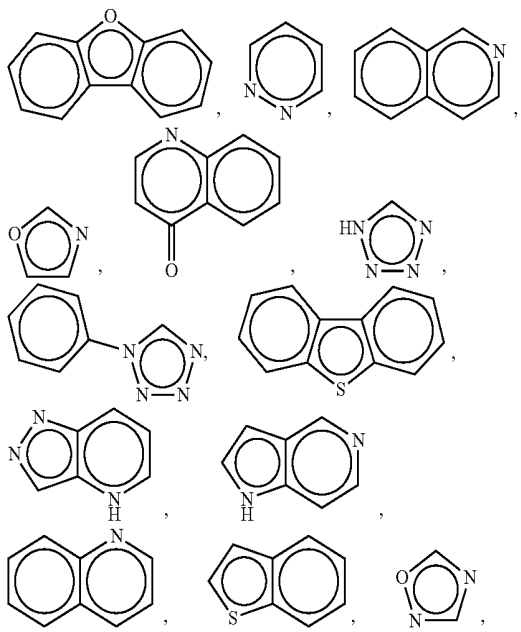


and wherein the moiety D can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0090] In a ninth aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety A, for each occurrence independently, can be selected from List A1.

List A1

[0091]



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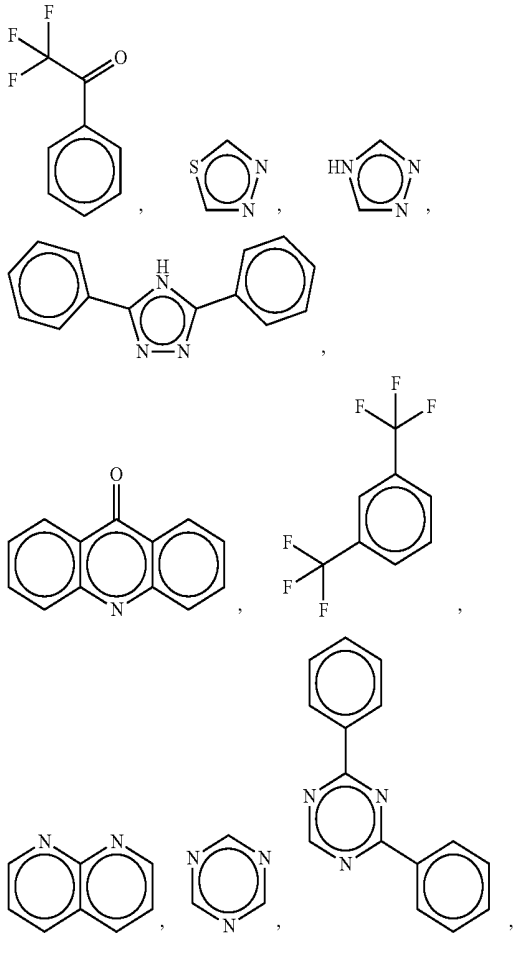

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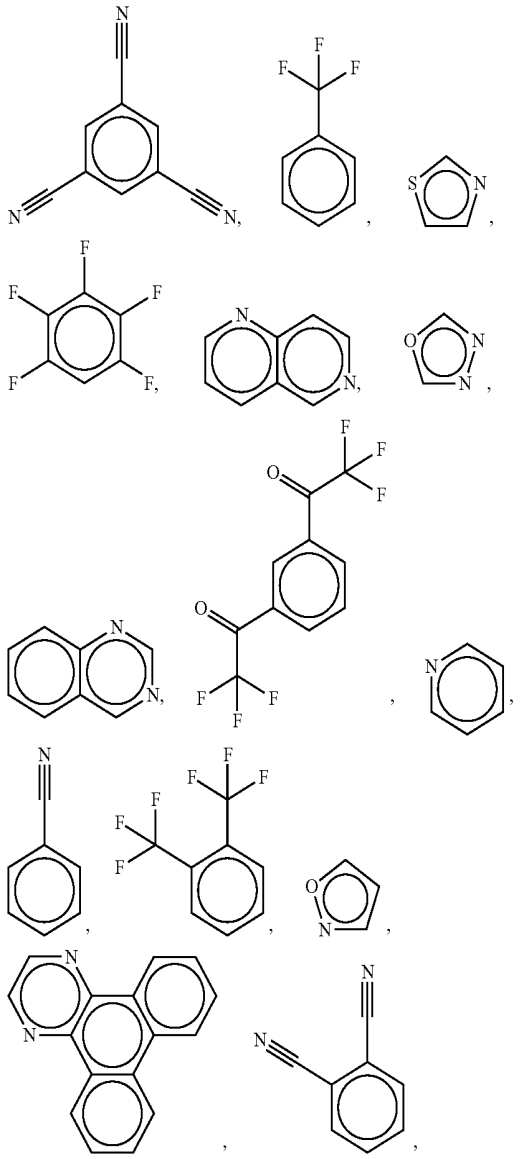

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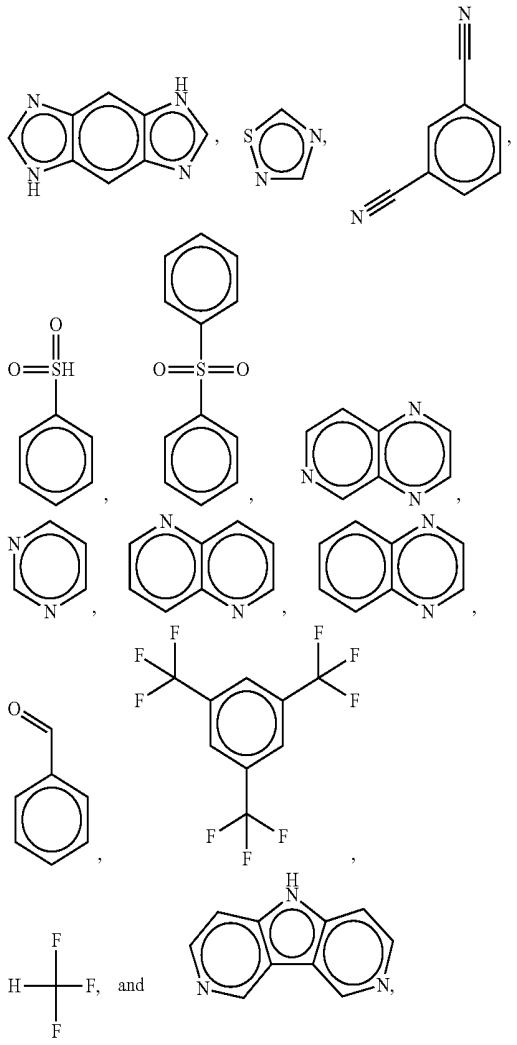
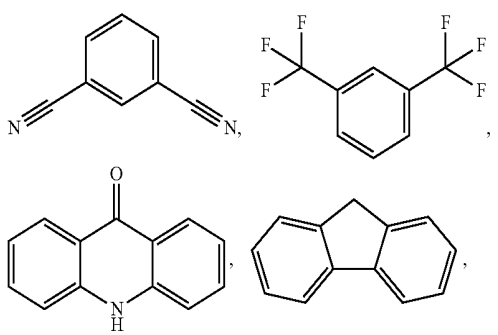


and wherein the moiety A can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0092] In a tenth aspect, the present invention is a molecule as defined above with respect to the first, second, third, aspects of the present invention, and wherein the moiety A, for each occurrence independently, can be selected from List A1, List A2, or both.

List A2

[0093]



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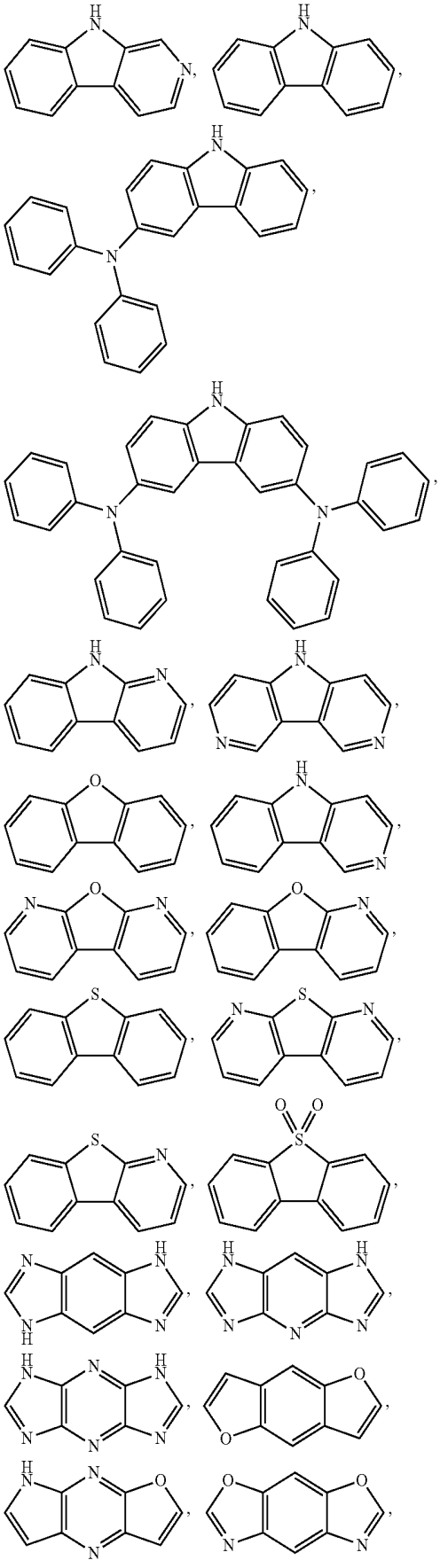

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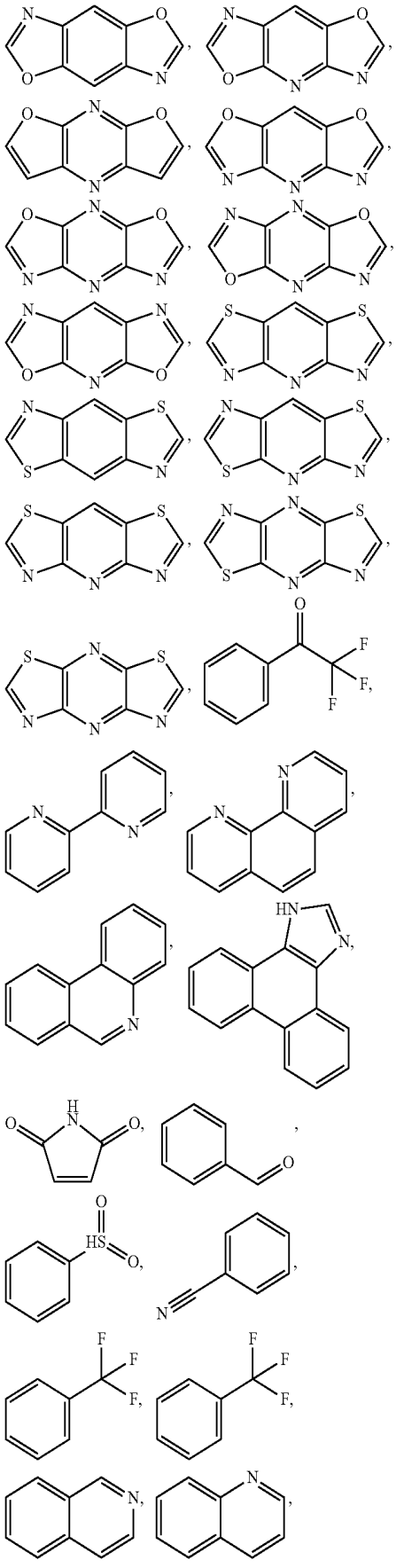

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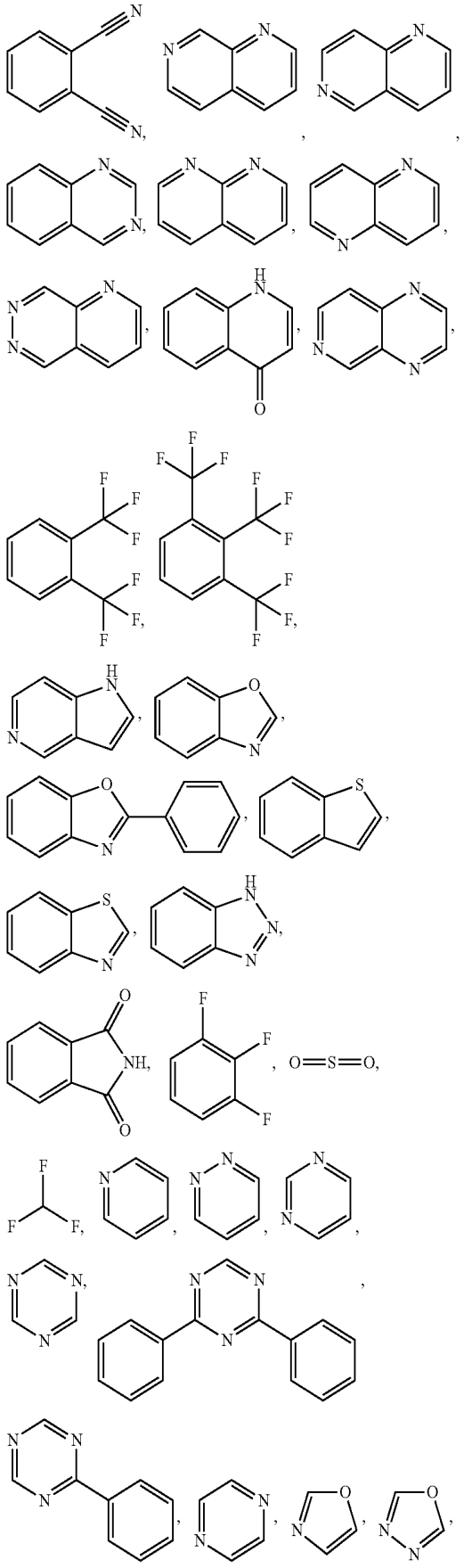

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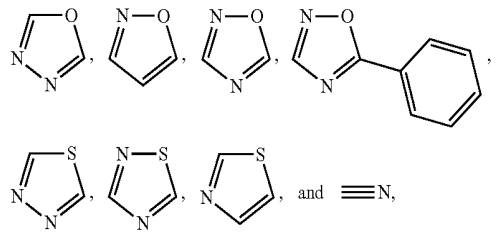
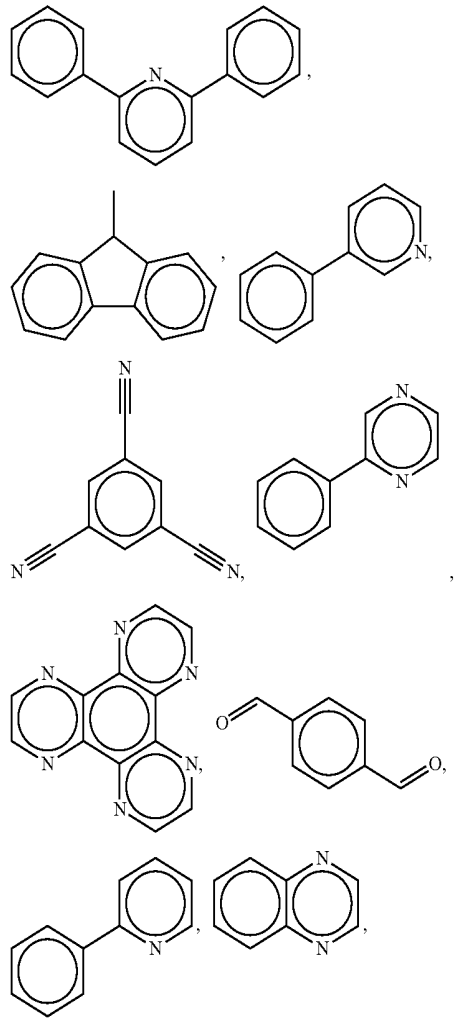


and wherein the moiety A can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0094] In a eleventh aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety A, for each occurrence independently, can be selected from List A1, List A2, List A3, or any combination thereof.

List A3

[0095]



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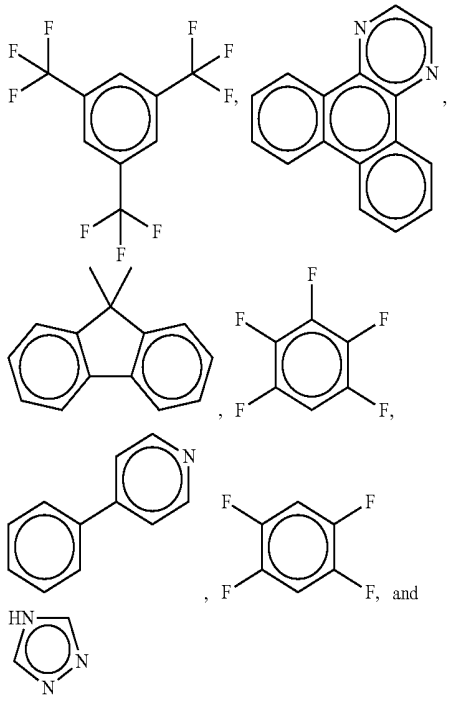
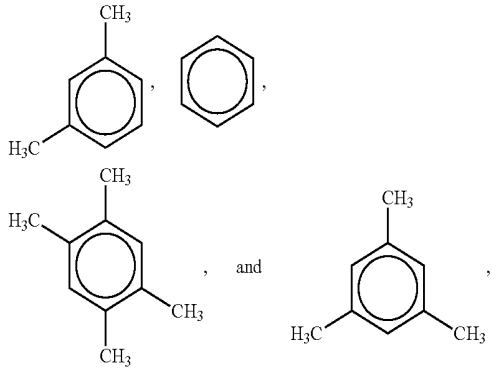


and wherein the moiety A can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0096] In a twelfth aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety B, for each occurrence independently, can be selected from List B1:

List B 1

[0097]

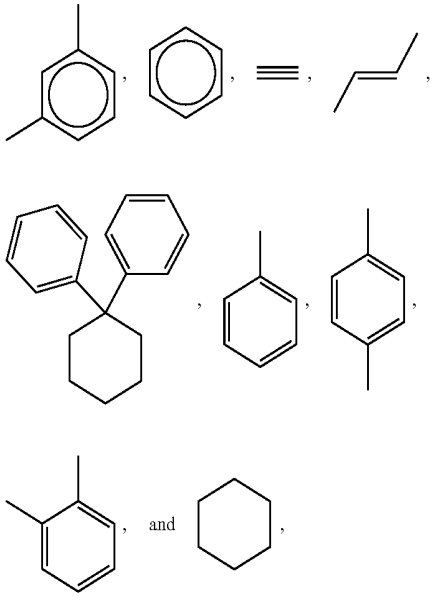


and wherein the moiety B can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0098] In a thirteenth aspect, the present invention is a molecule as defined above with respect to the first or second aspects of the present invention, and wherein the moiety B, for each occurrence independently, can be selected from List B1, List B2, or both.

List B2

[0099]

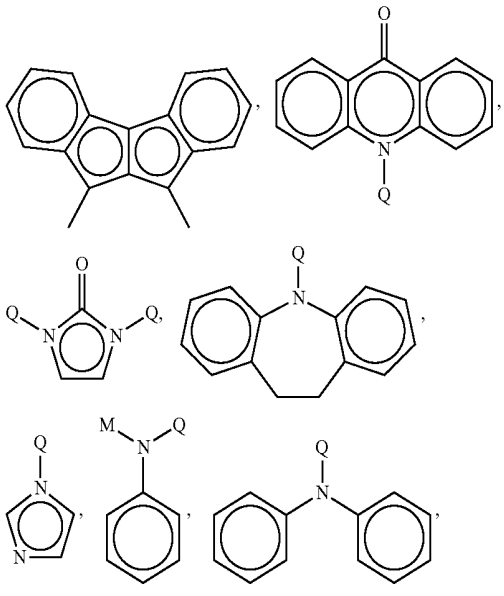


and wherein the moiety B can be optionally substituted as described above with respect to the third, fourth, and fifth aspects of the present invention.

[0100] In an example embodiment of the sixth aspect of the present invention, the moiety D, for each occurrence independently, is selected from List D4.

List D4

[0101]



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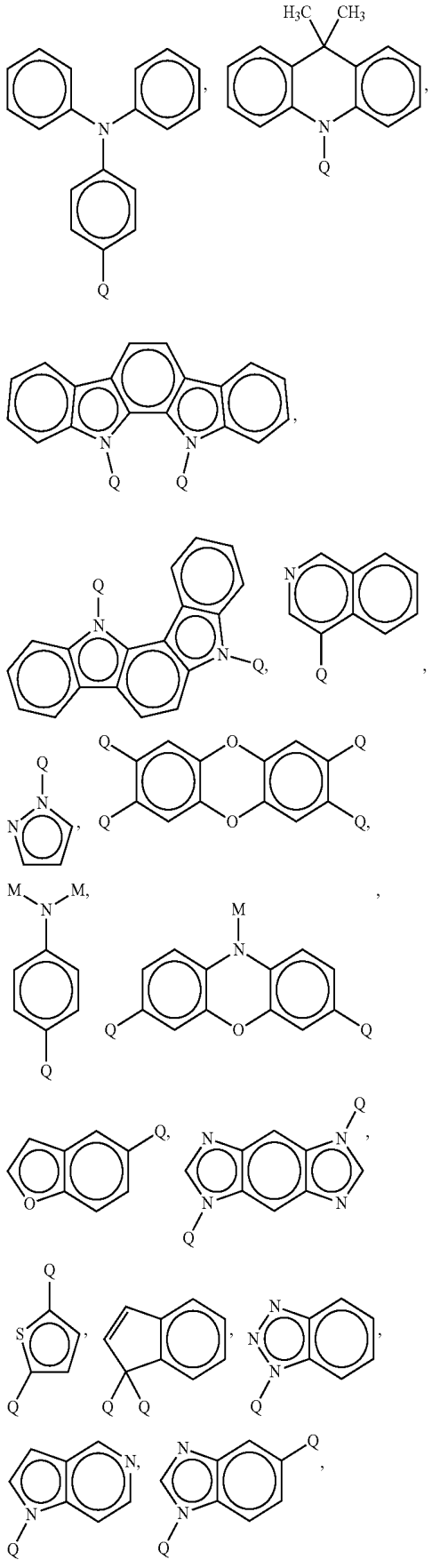

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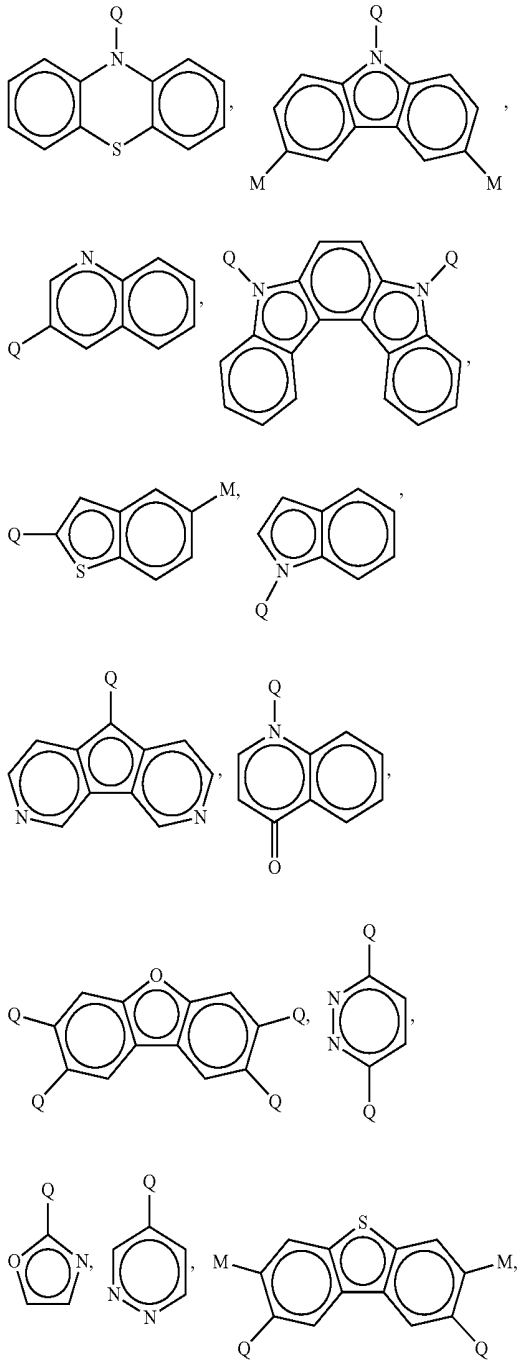

wherein, within each molecule:

[0102] Q is the moiety A or a moiety B_{0-2}-A and each M is the moiety A or the moiety B_{0-2}-A,

[0103] all groups Q are the same and all groups M are the same, and each group Q is the same or different from any group M, and the moieties A and B are defined above with respect to the first, second, and third aspects of the present invention.

[0104] In an example embodiment of the seventh aspect of the present invention, the moiety D, for each occurrence independently, is selected from List D4, List D5, or both.

List D5

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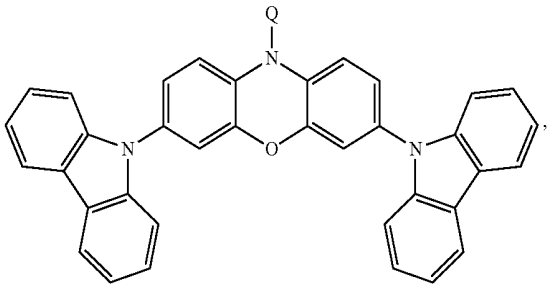
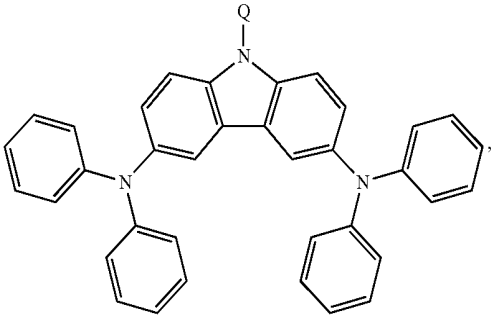
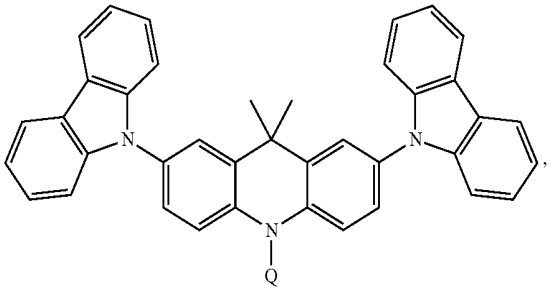
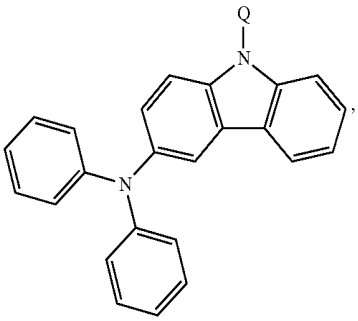
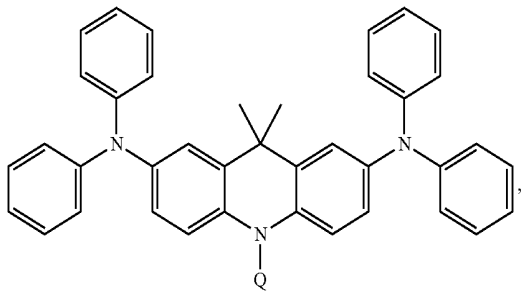
[0105]

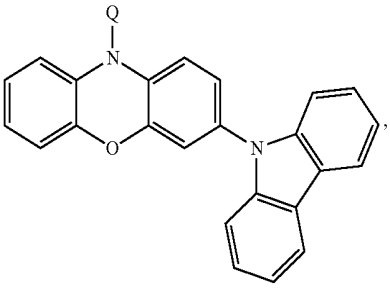


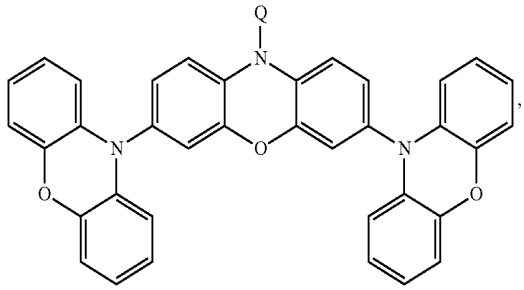


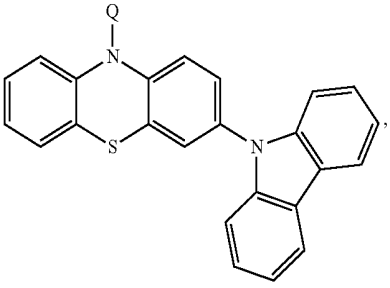


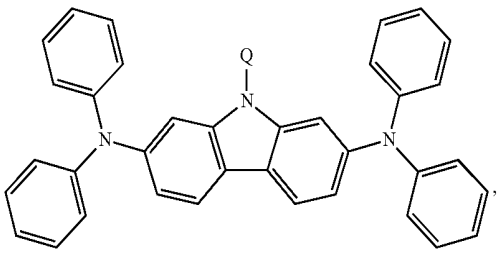


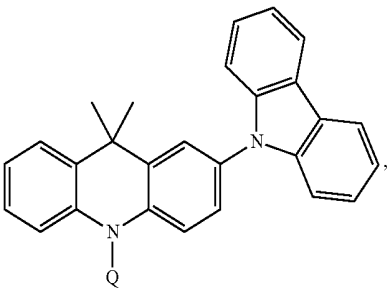












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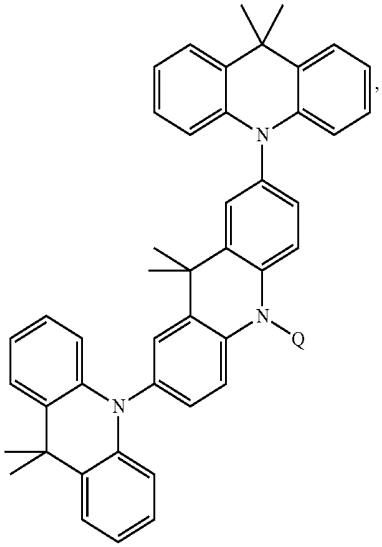

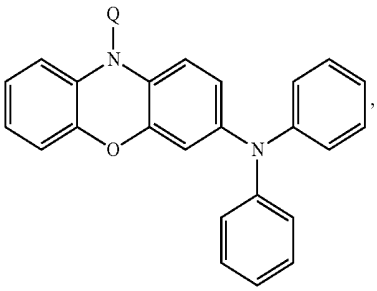

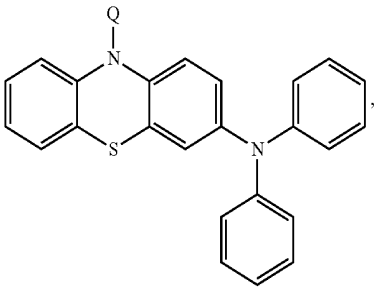

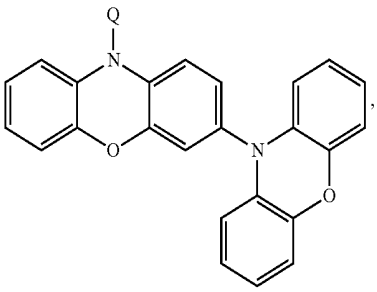

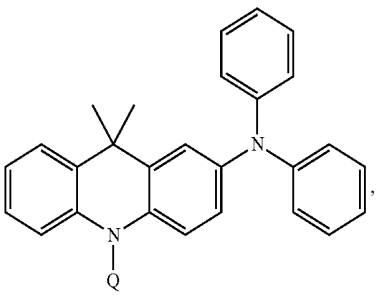

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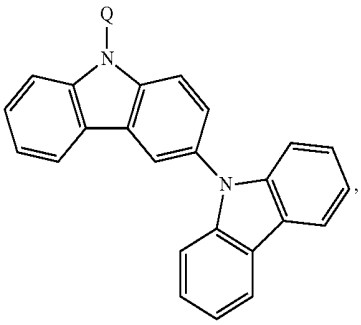

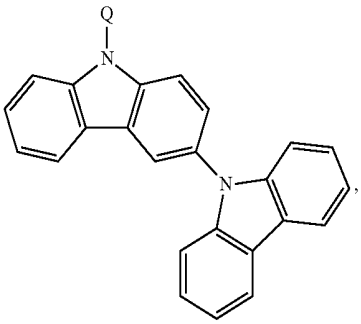

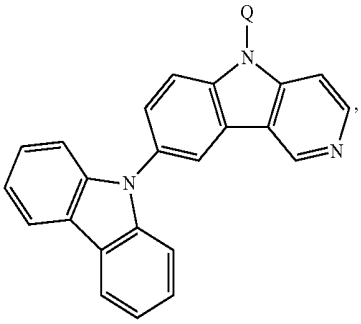

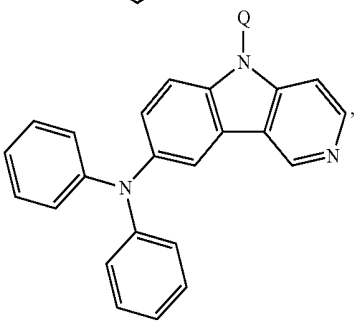

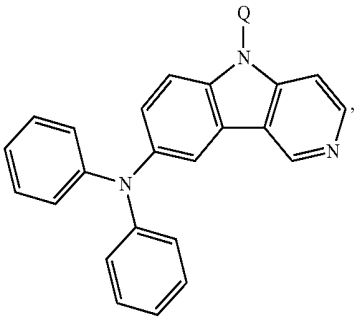

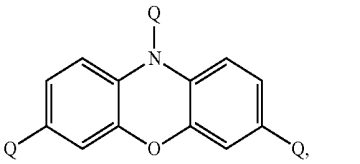

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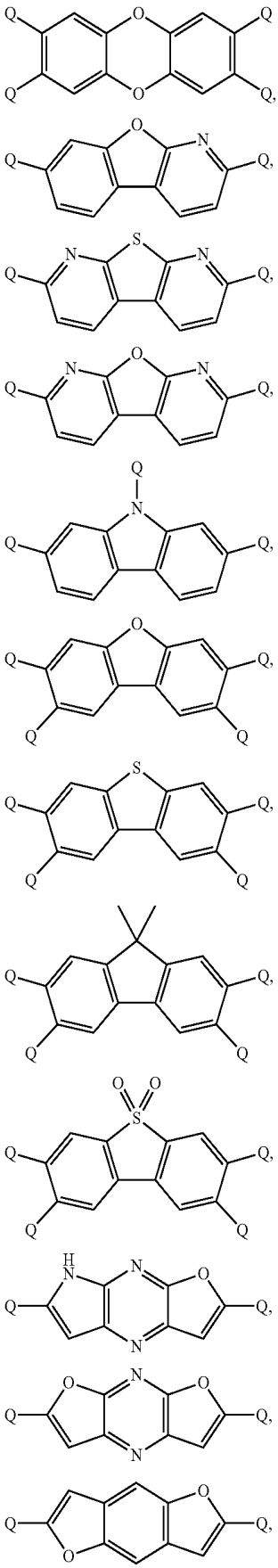

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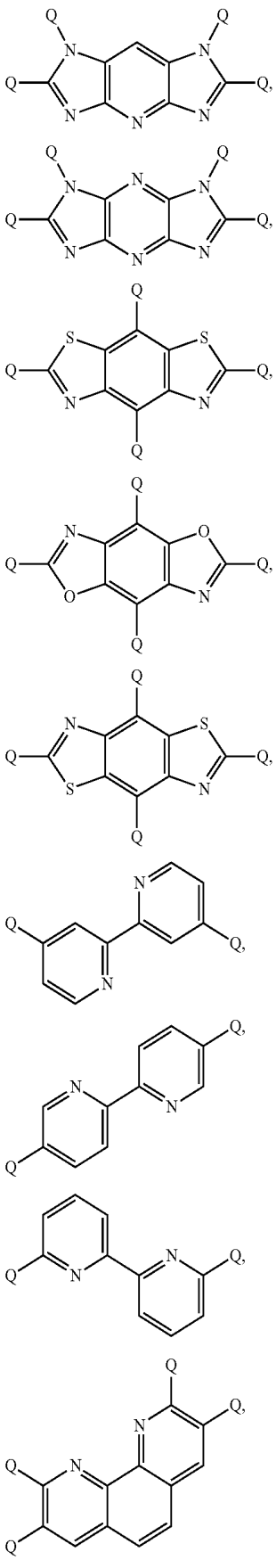

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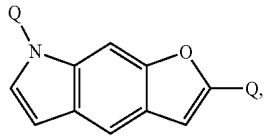

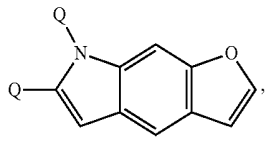

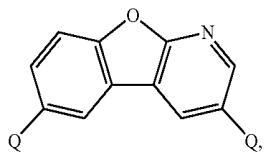

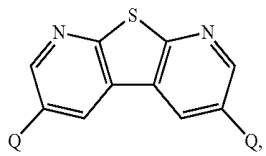

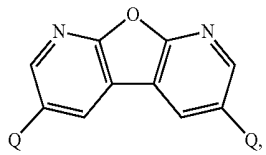

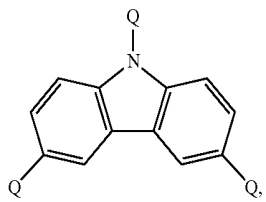

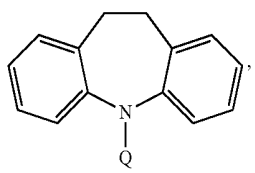

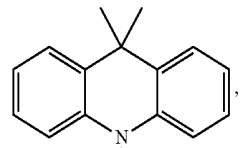

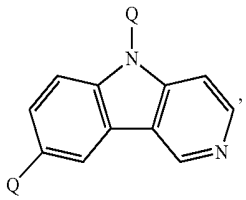

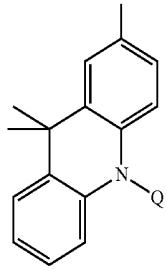

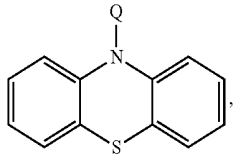

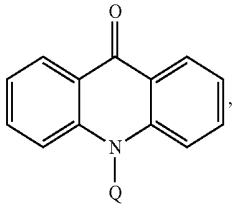

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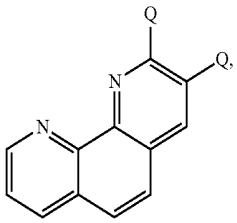

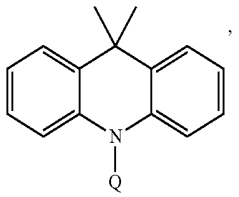

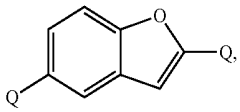

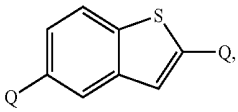

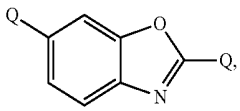

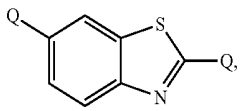

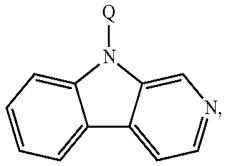

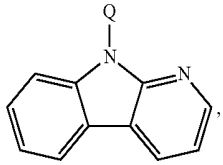

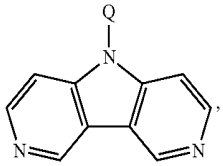

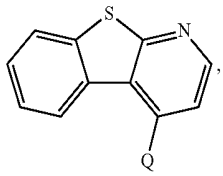

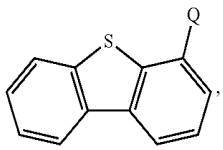

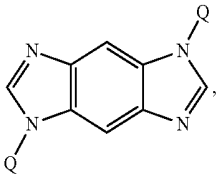

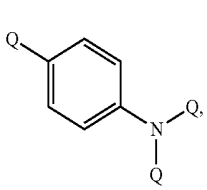

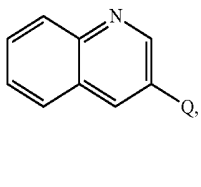

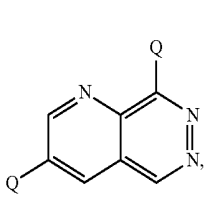

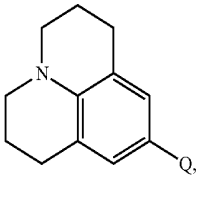

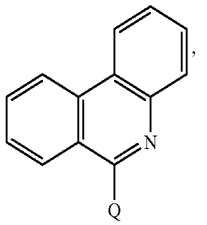

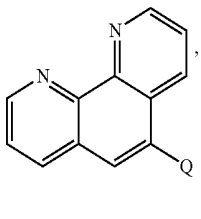

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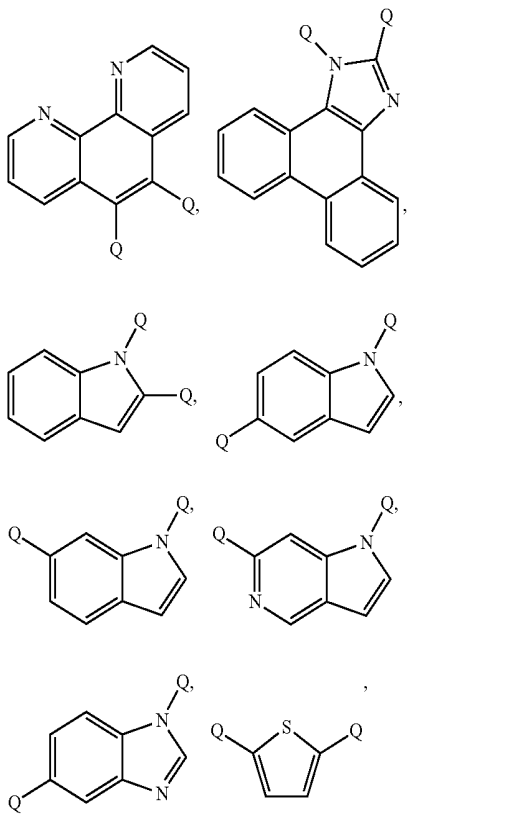

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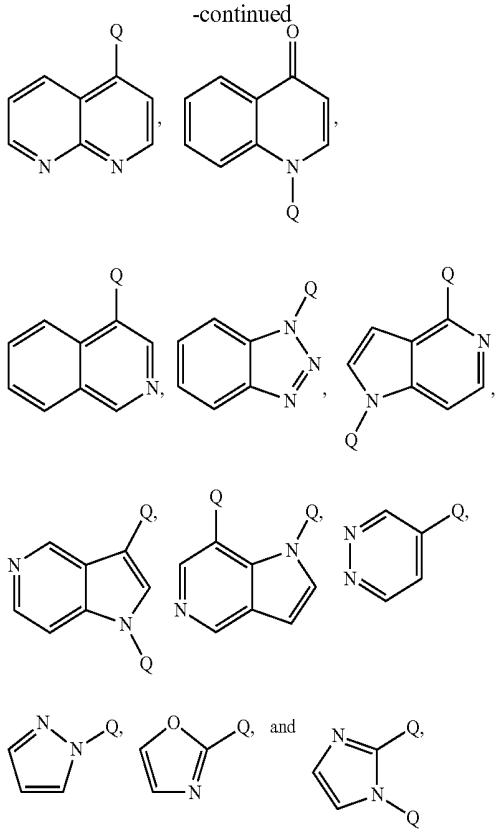


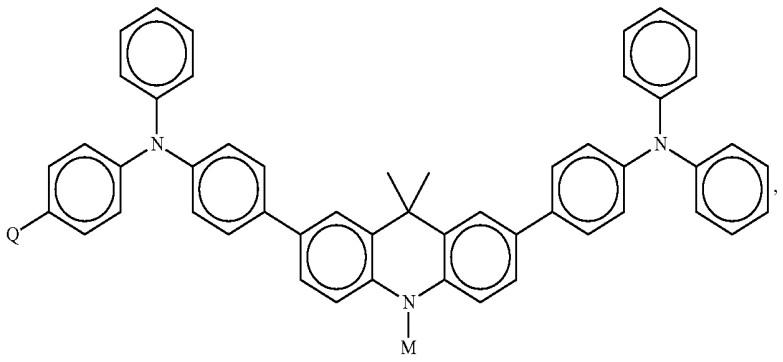
wherein, within each molecule:

[0106] Q is independently selected from the group consisting of the moiety A, a moiety B_{0-2}-A, H, C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, (5-20 atom) heteroaryl, and —N(C_6-C_{18} aryl)$_2$, and wherein the moieties A and B are defined above with respect to the first, second, and third aspects of the present invention.

[0107] In an example embodiment of the seventh and eighth aspects of the present invention, the moiety D, for each occurrence independently, can also be selected from List D6.

List D6

[0108]



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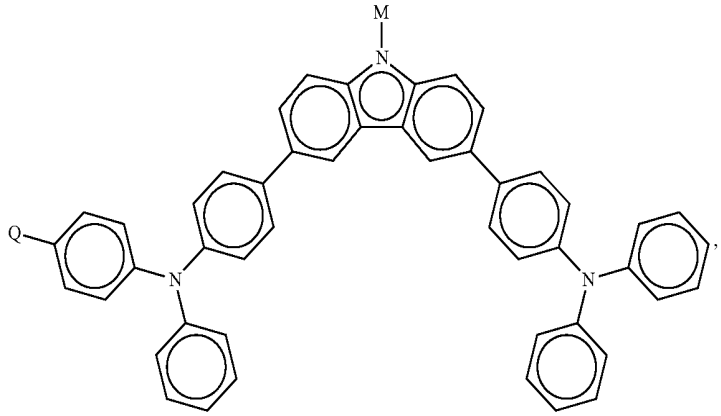

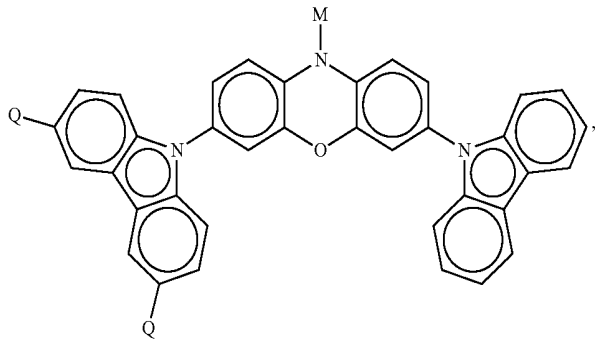

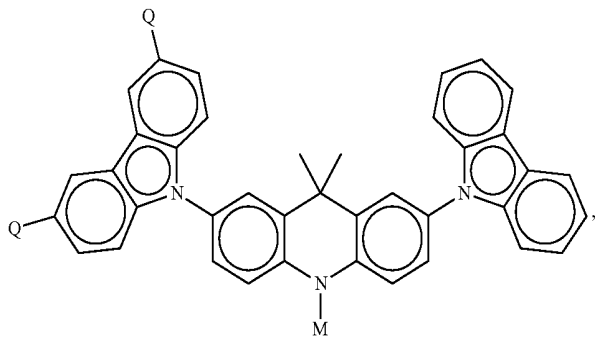

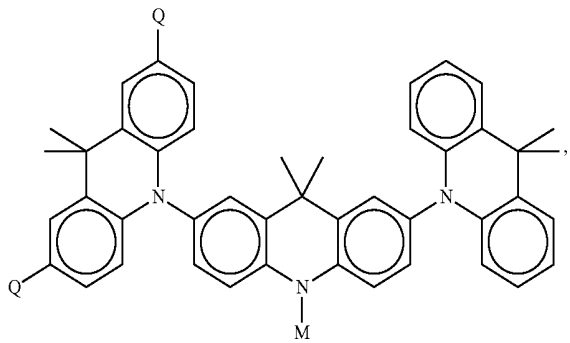

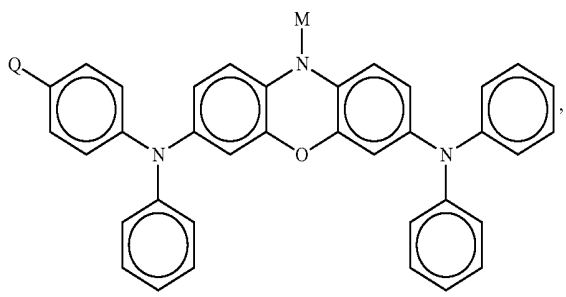

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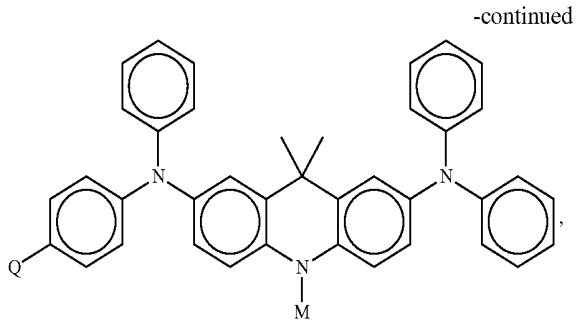

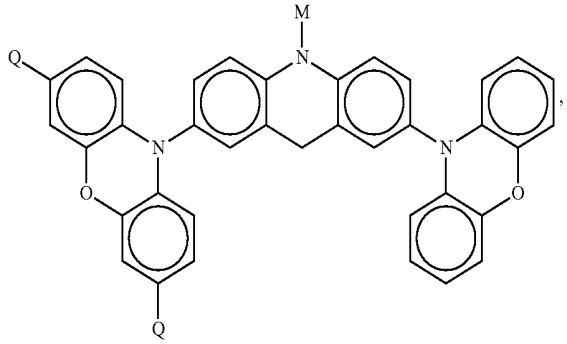

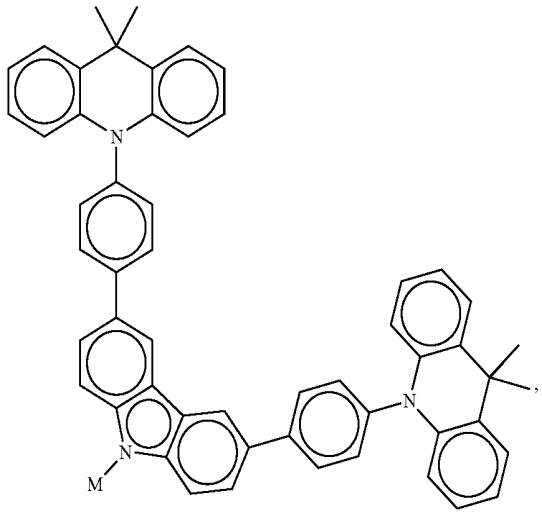

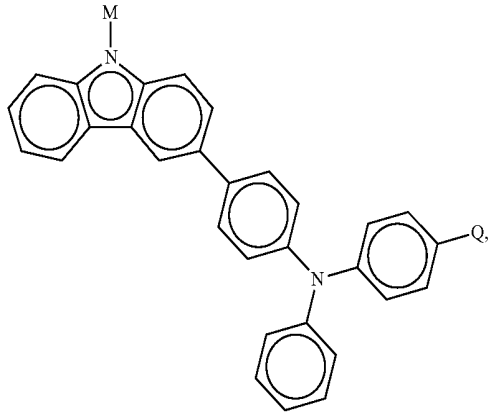

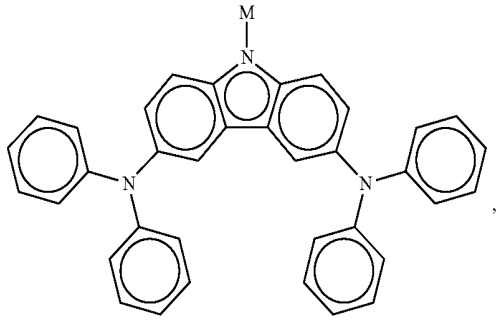

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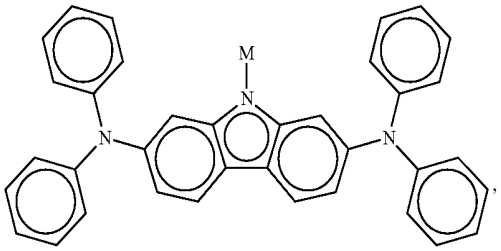

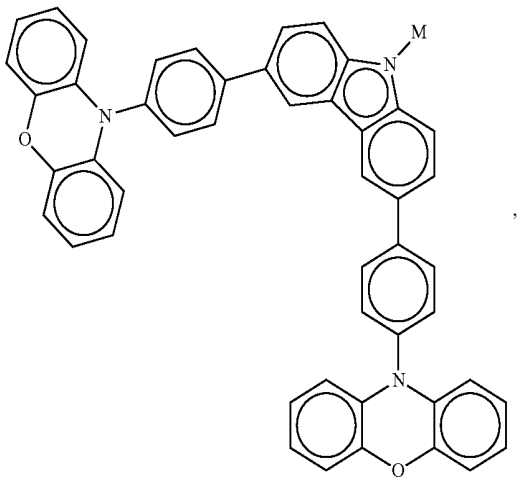

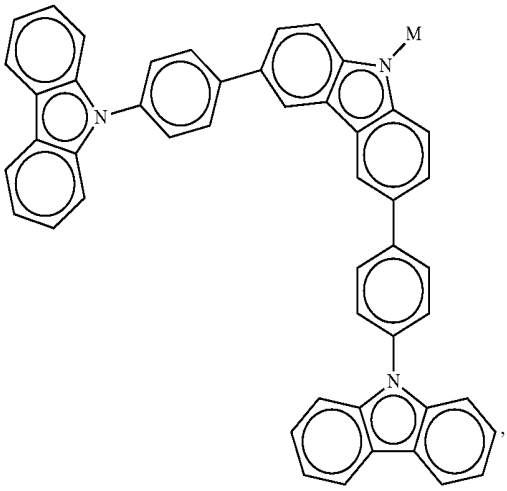

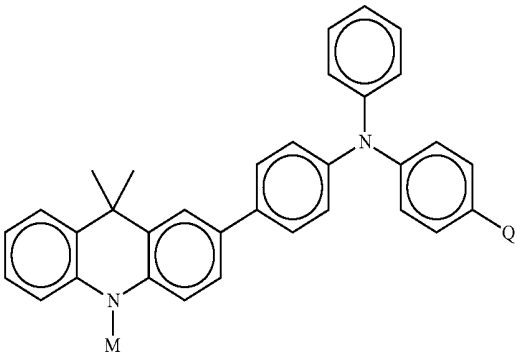

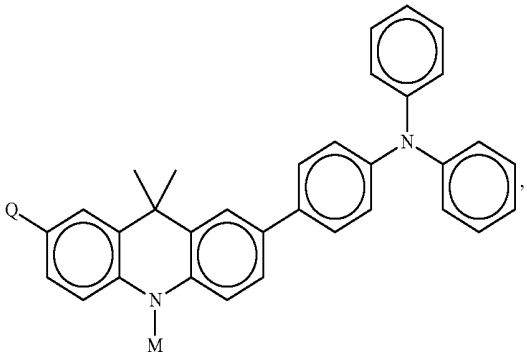

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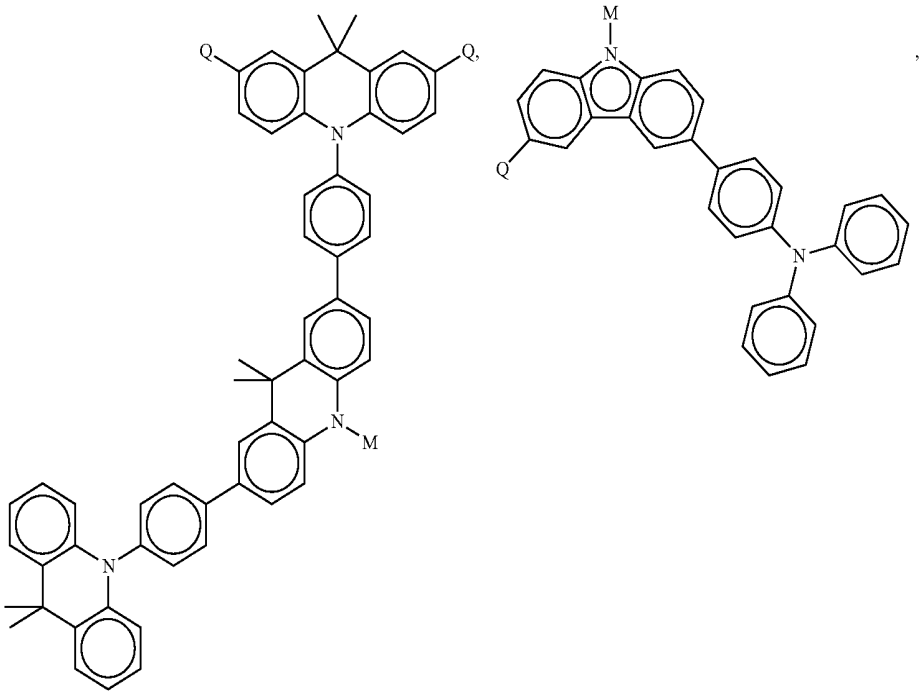

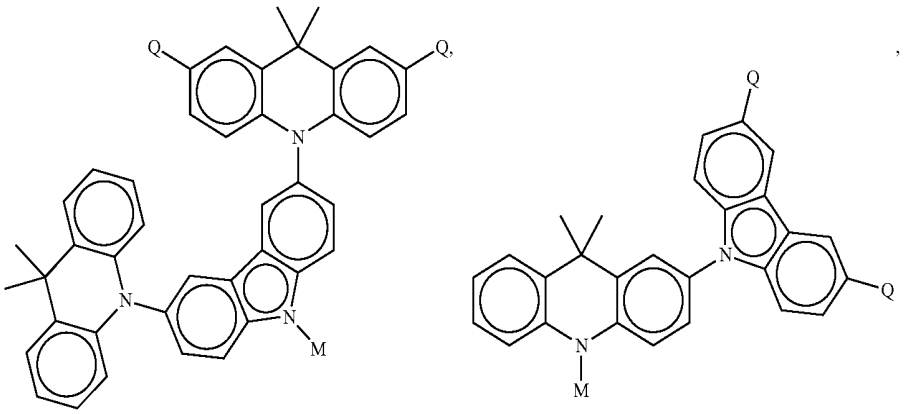

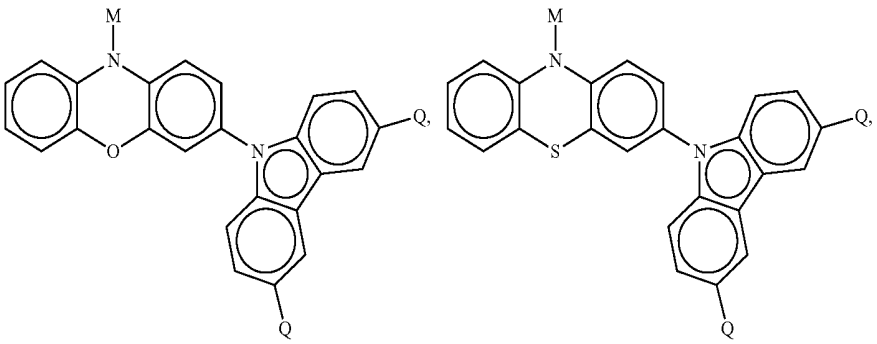

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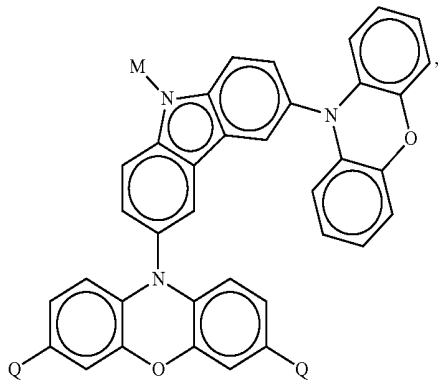

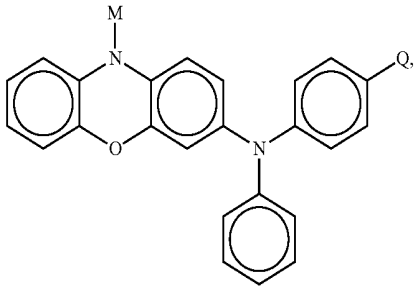

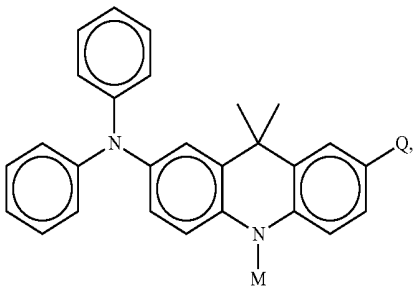

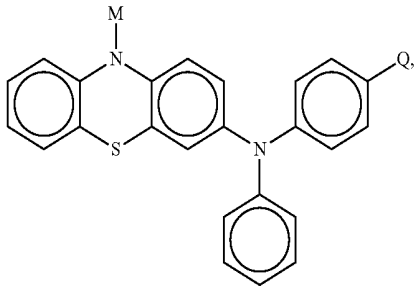

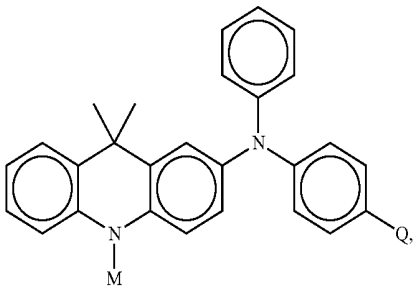

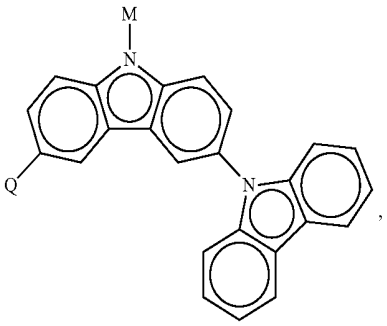

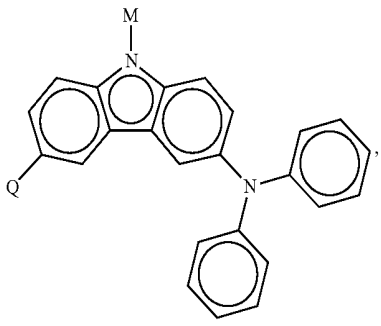

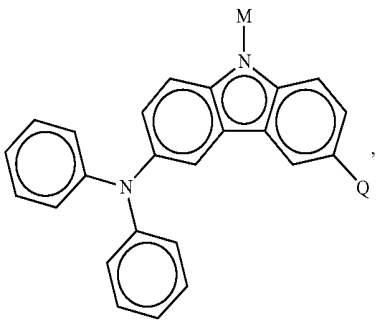

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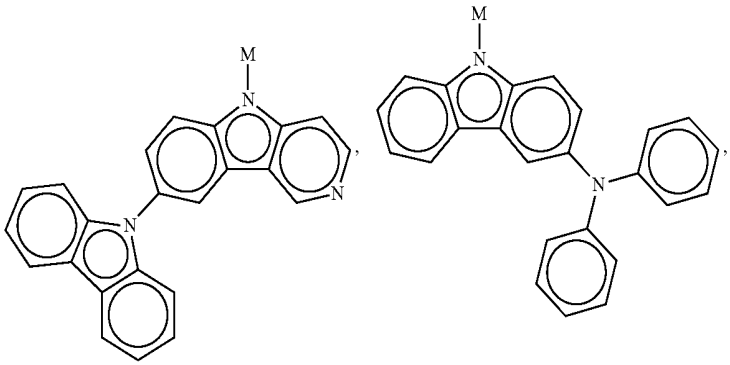

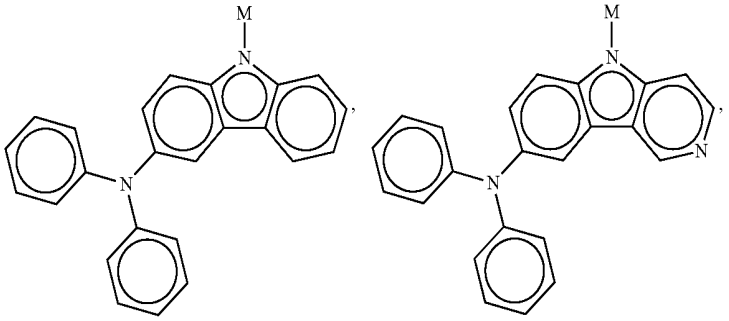

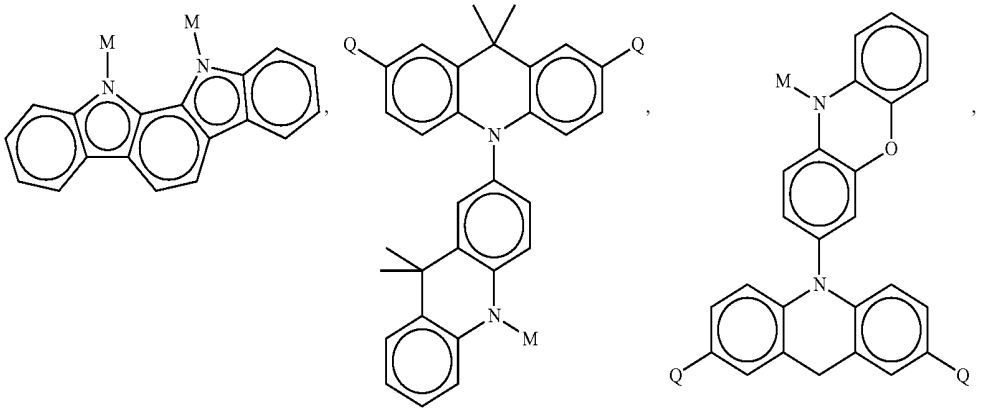

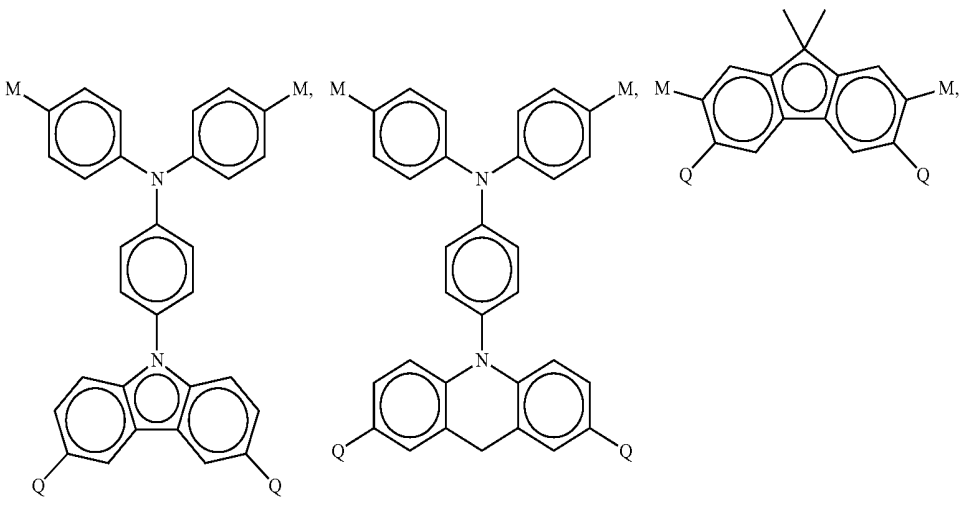

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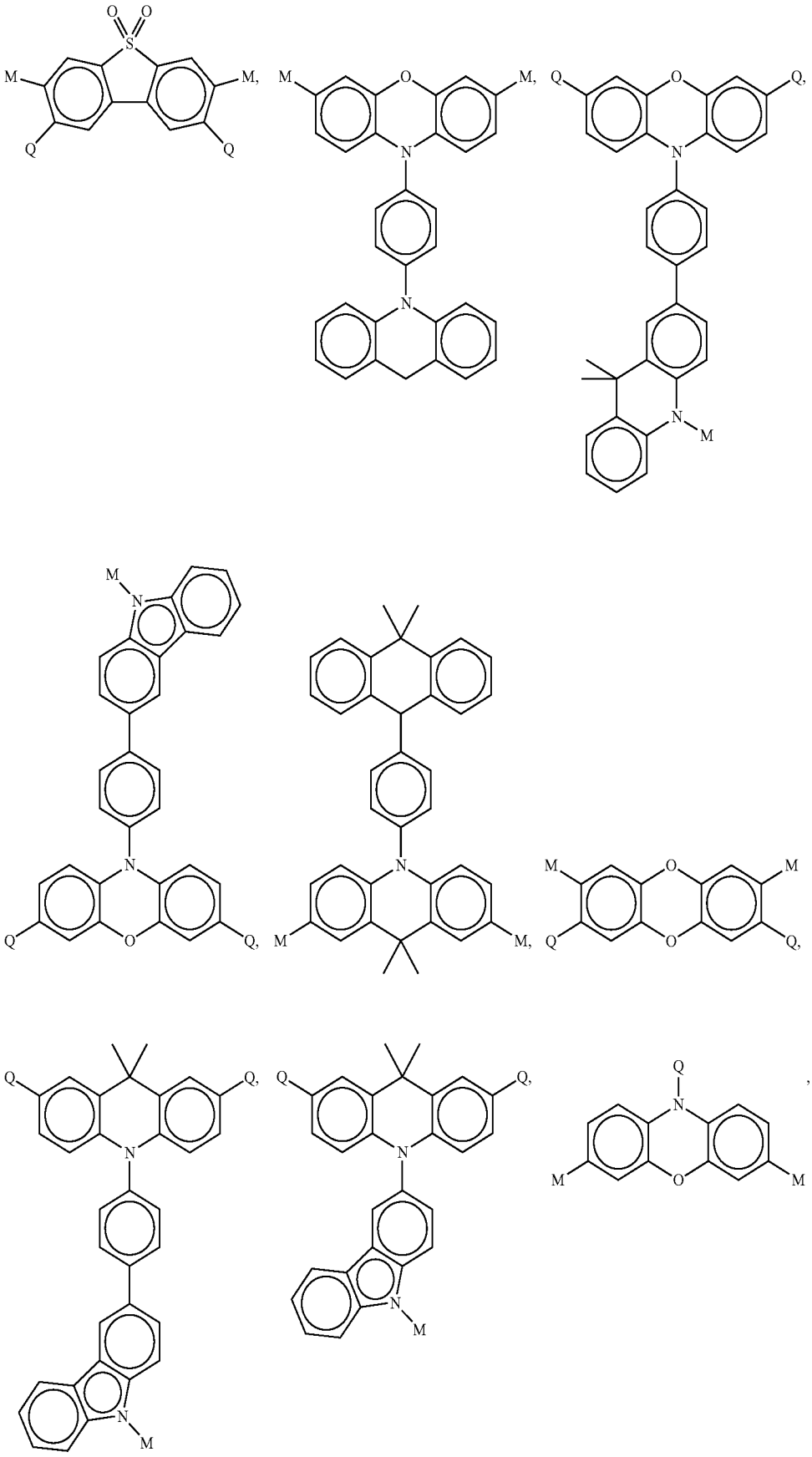

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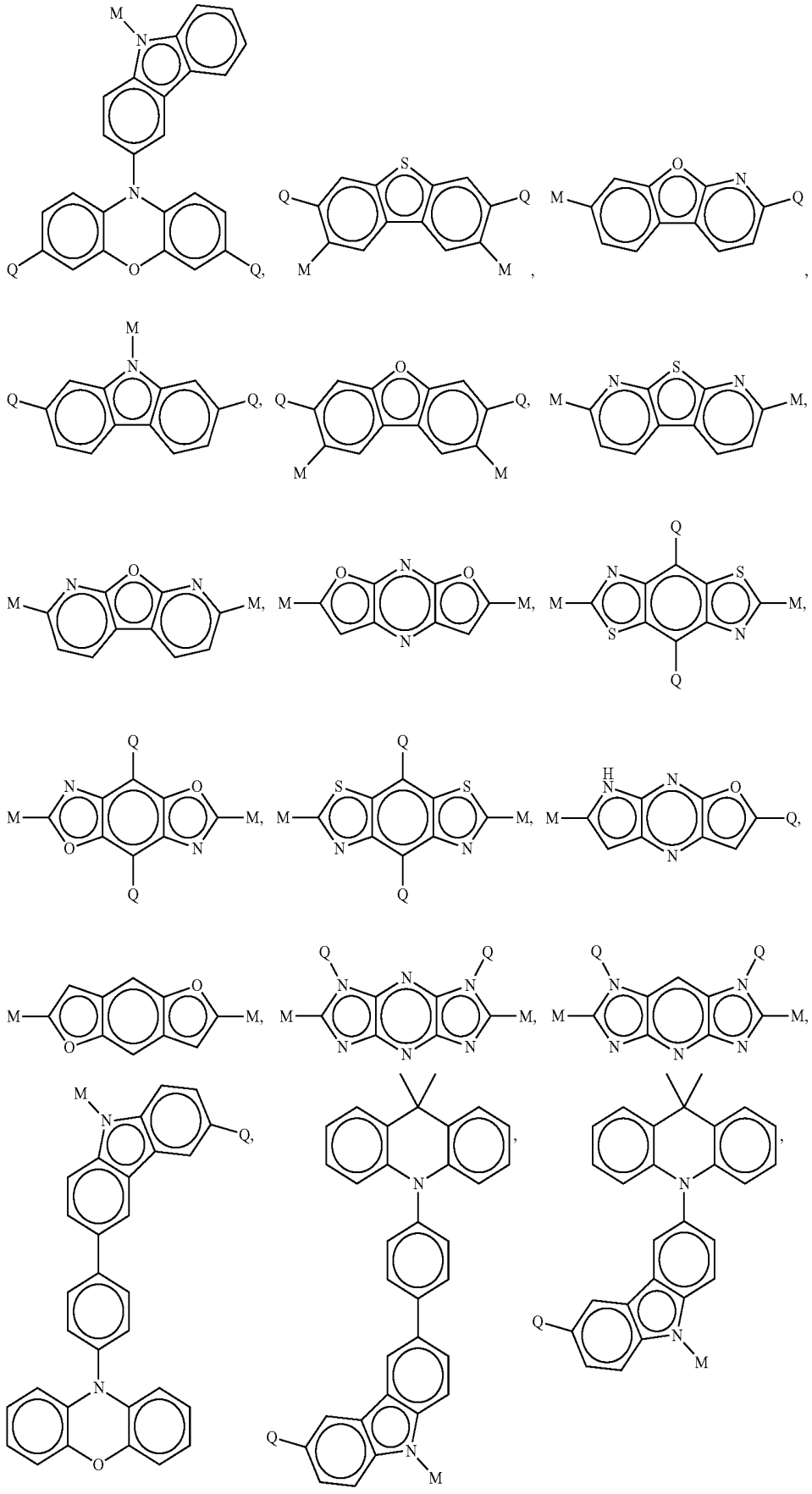

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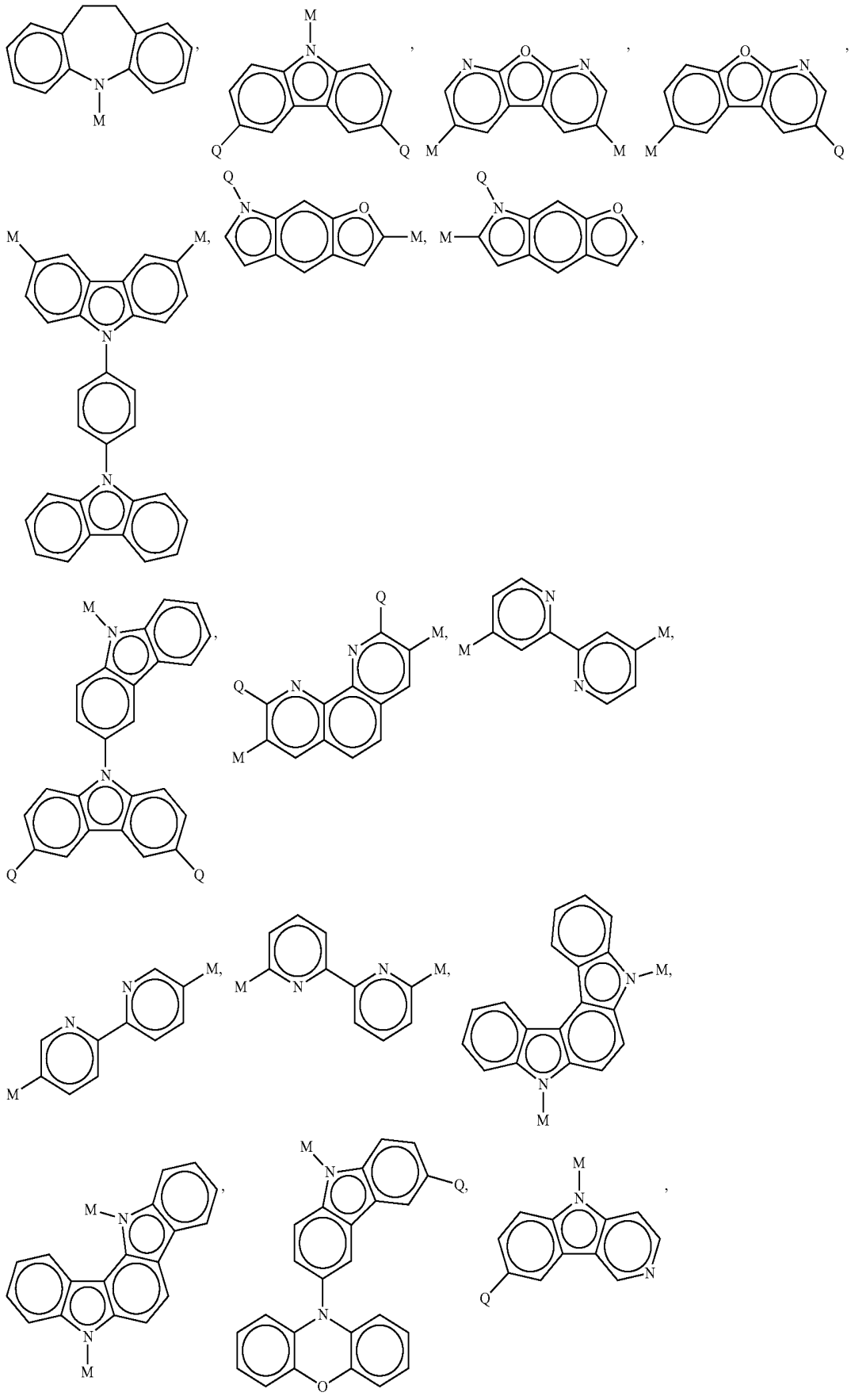

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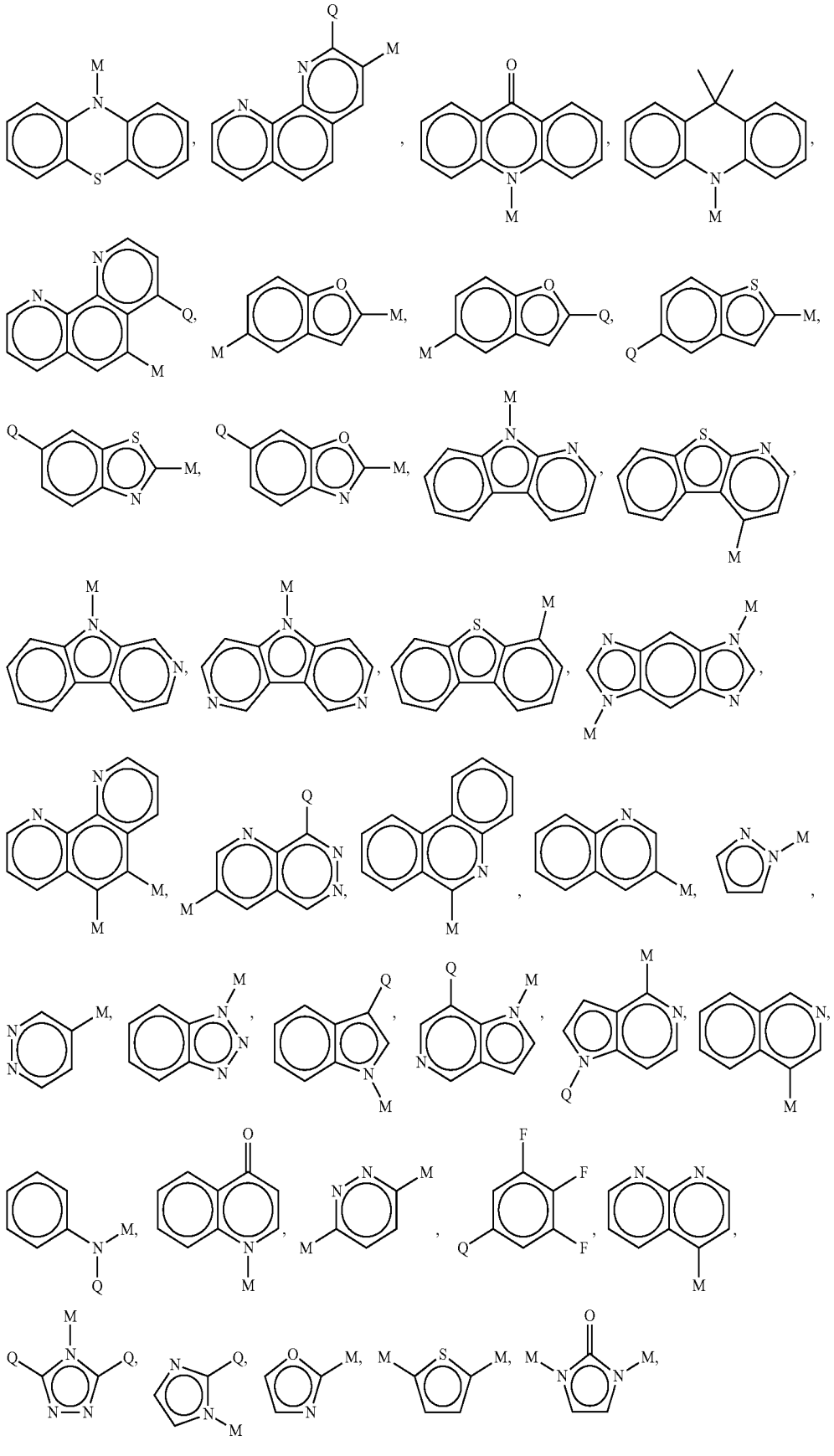

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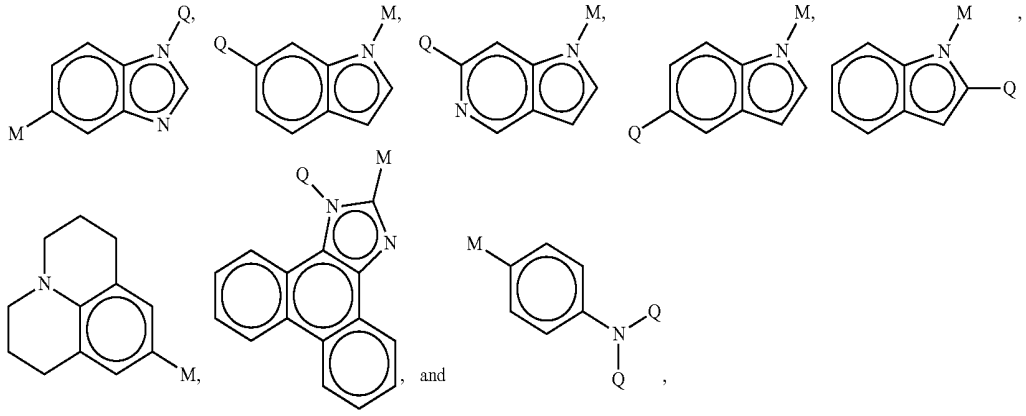


wherein, within each molecule:

[0109] Q is independently selected from the group consisting of the moiety A, a moiety B_{0-2}-A, H, C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, (5-20 atom) heteroaryl, and —N(C_6-C_{18} aryl)$_2$,

[0110] M is independently selected from the group consisting of the moiety A, a moiety B_{0-2}-A, H, C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, (5-20 atom) heteroaryl, and —N(C_6-C_{18} aryl)$_2$,

[0111] at least one of Q and M is the moiety B_{0-2}-A,

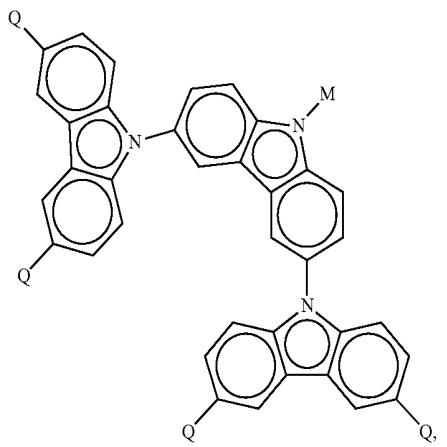
[0112] all groups Q are the same and all groups M are the same, and

[0113] each group Q is the same or different from any group M, and wherein the moieties A and B are defined above with respect to the first, second, and third aspects of the present invention.

[0114] In an example embodiment of the seventh and eighth aspects of the present invention, the moiety D, for each occurrence independently, can also be selected from List DN2.

List DN2

[0115]



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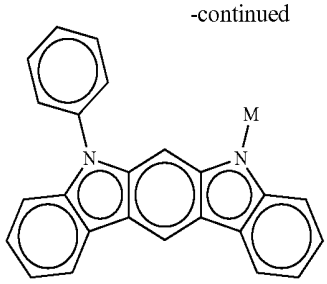


wherein, within each molecule:

[0116] Q is independently selected from the group consisting of the moiety A, a moiety B_{0-2}-A, H, C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, (5-20 atom) heteroaryl, and —N(C_6-C_{18} aryl)$_2$,

[0117] M is independently selected from the group consisting of the moiety A, a moiety B_{0-2}-A, H, C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, (5-20 atom) heteroaryl, and —N(C_6-C_{18} aryl)$_2$,

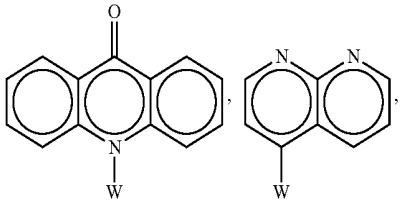
[0118] at least one of Q and M is the moiety B_{0-2}-A,

[0119] all groups Q are the same and all groups M are the same, and each group Q is the same or different from any group M, and wherein the moieties A and B are defined above with respect to the first, second, and third aspects of the present invention.

[0120] In an example embodiment of the ninth aspect of the present invention, the moiety A, for each occurrence independently, is selected from List A4.

List A4

[0121]



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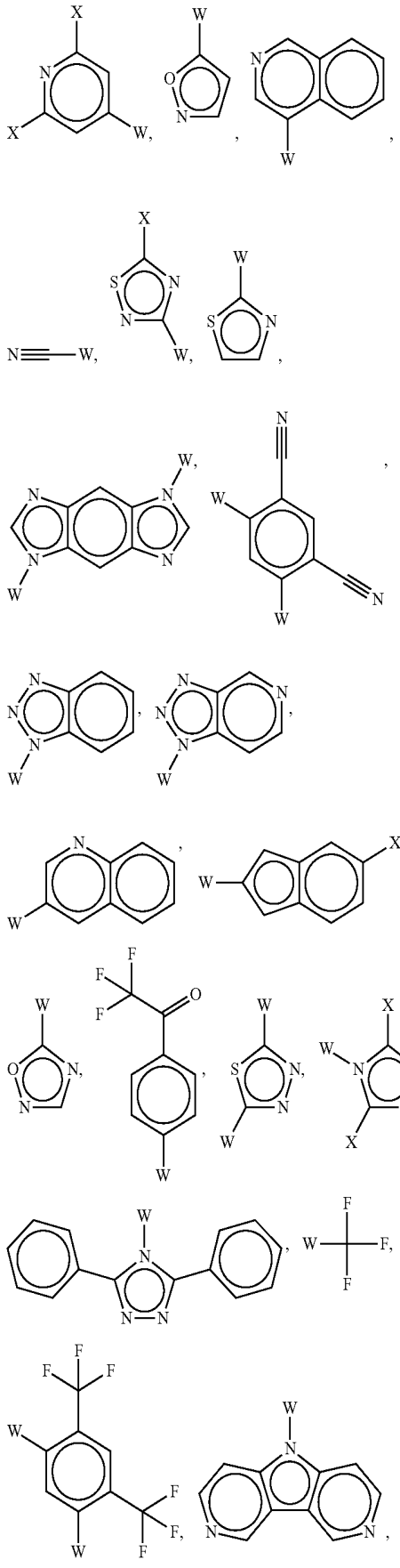

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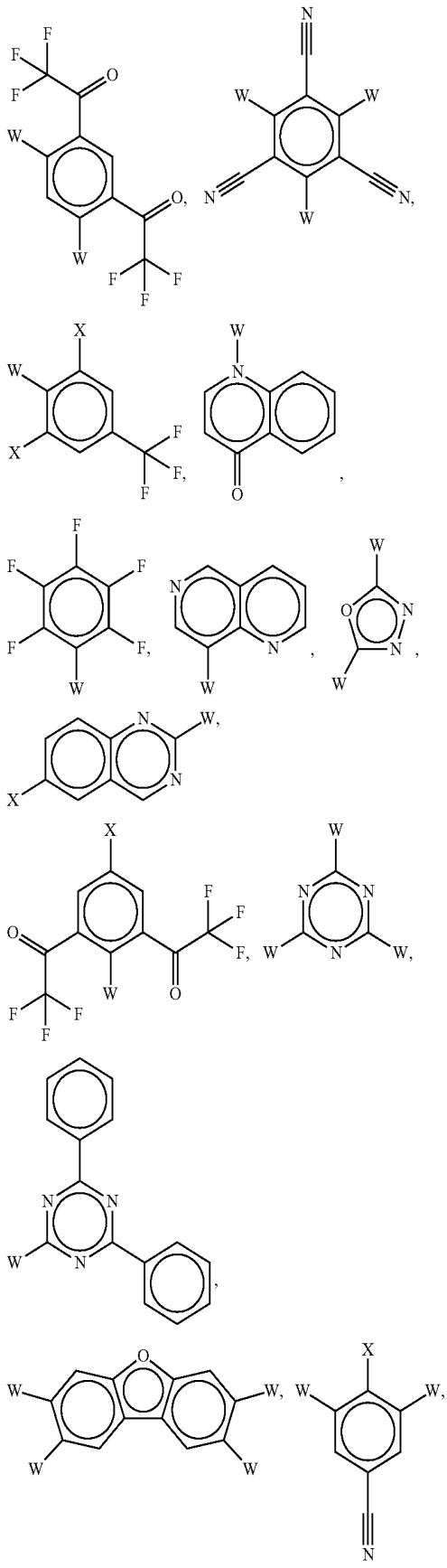

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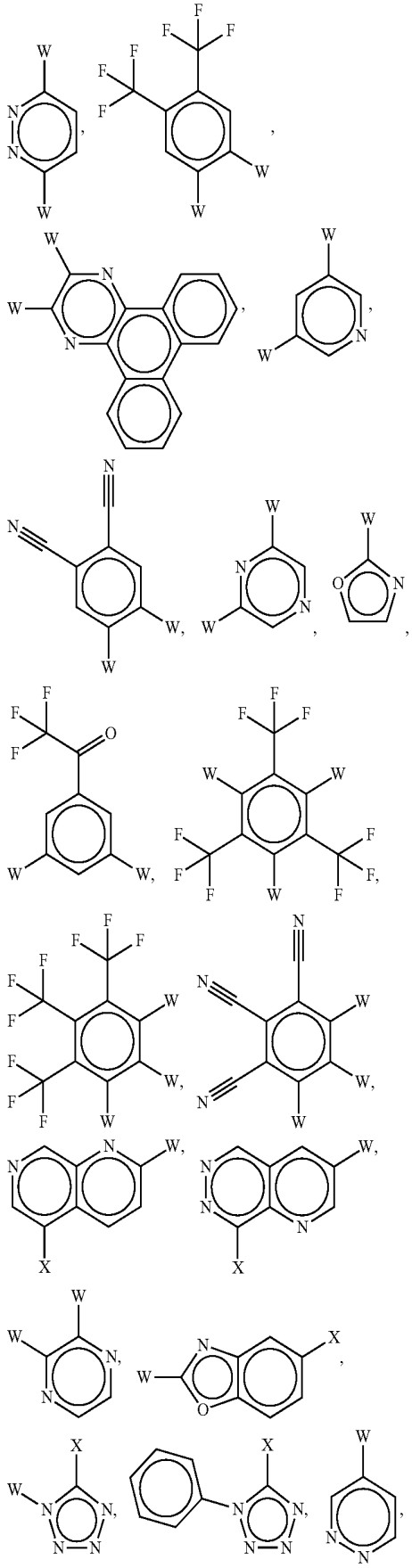

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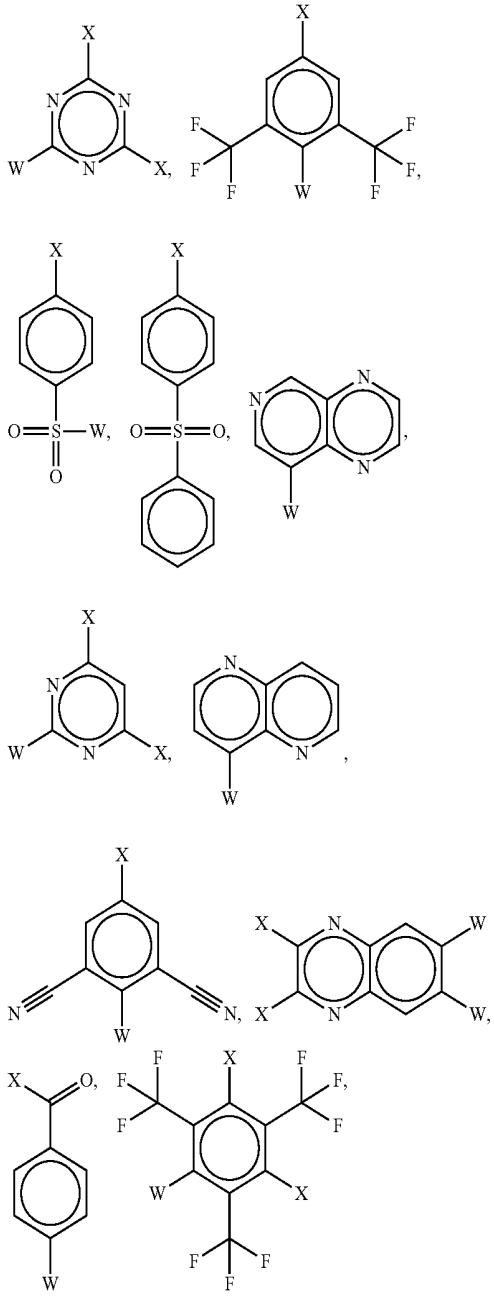


wherein, within each molecule:

[0122] W is the moiety D or a moiety B_{0-2}-D and each X is the moiety D or the moiety B_{0-2}-D,

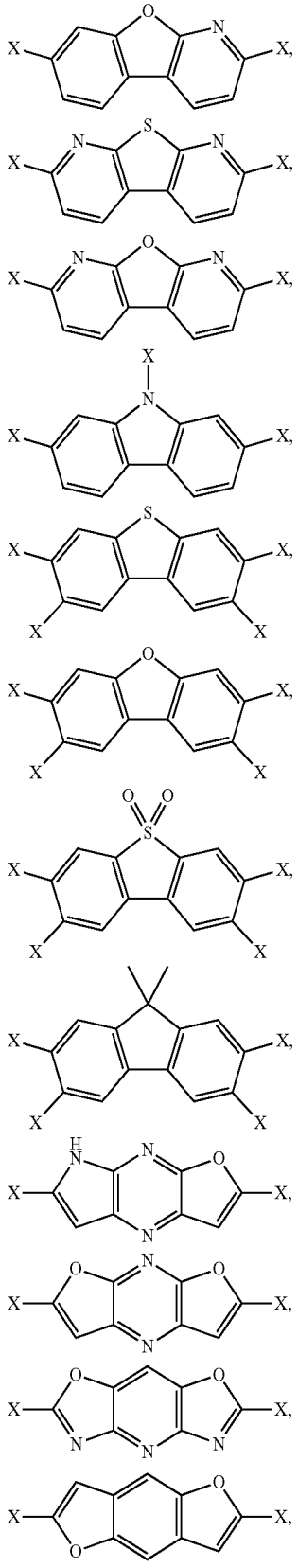
[0123] all groups W are the same and all groups X are the same, and

[0124] each group W is the same or different from any group X, and wherein the moieties D and B are defined above with respect to the first, second, and third aspects of the present invention.

[0125] In an example embodiment of the tenth aspect of the present invention, the moiety A, for each occurrence independently, can be selected from List A4, List A5, or both.

List A5

[0126]



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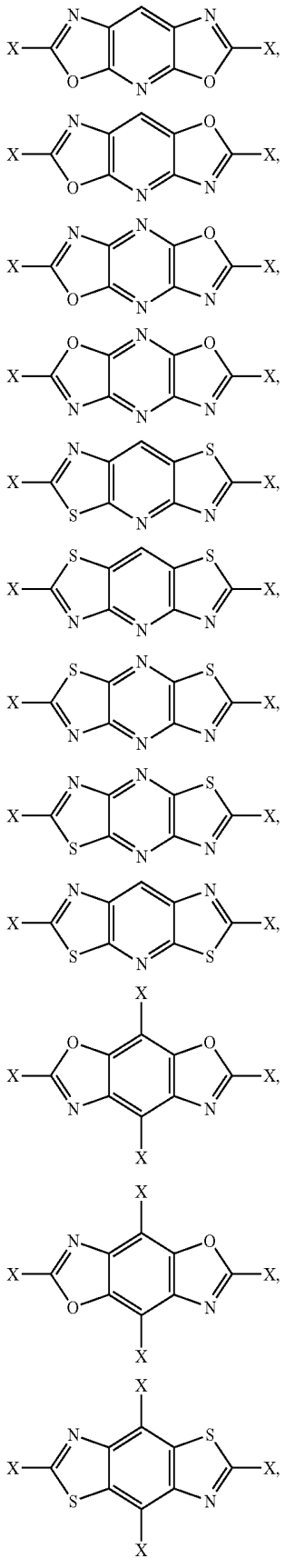

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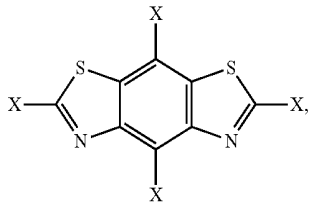

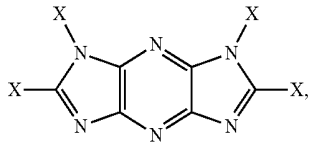

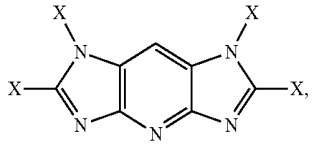

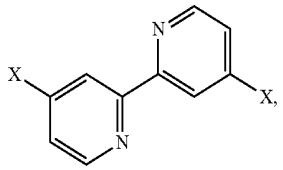

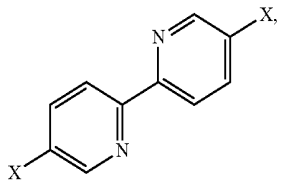

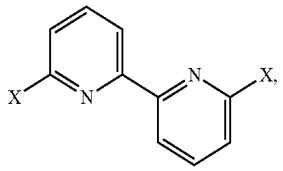

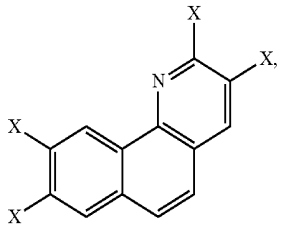

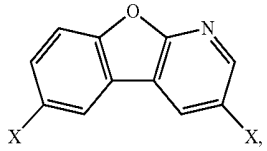

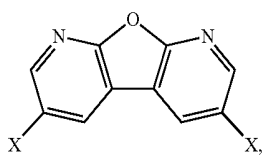

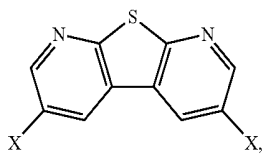

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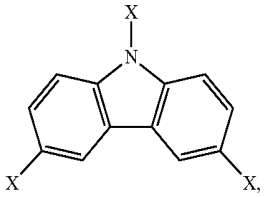

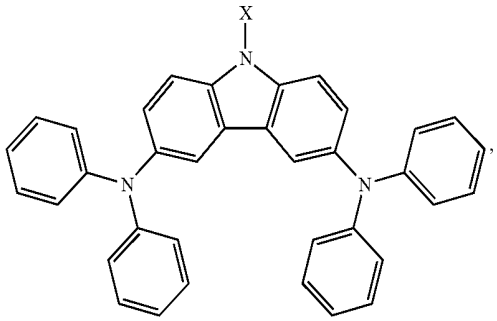

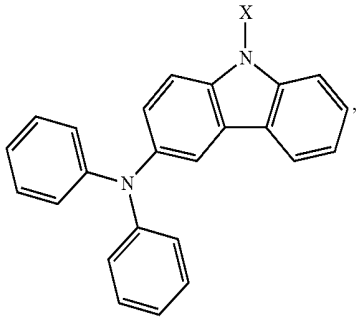

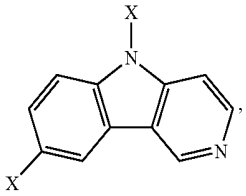

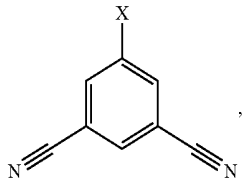

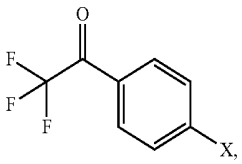

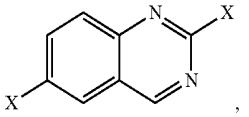

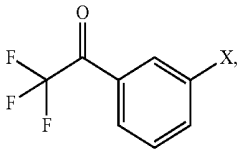

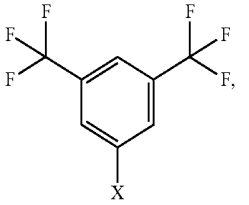

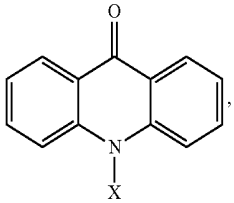

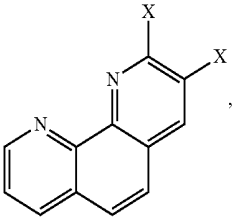

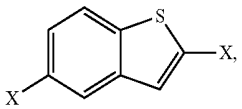

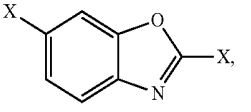

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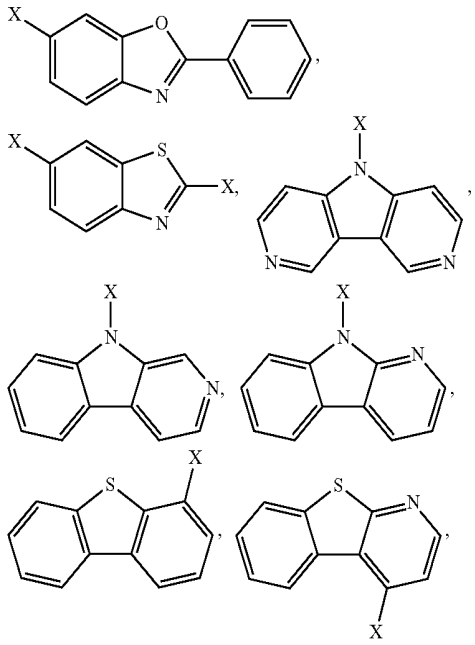

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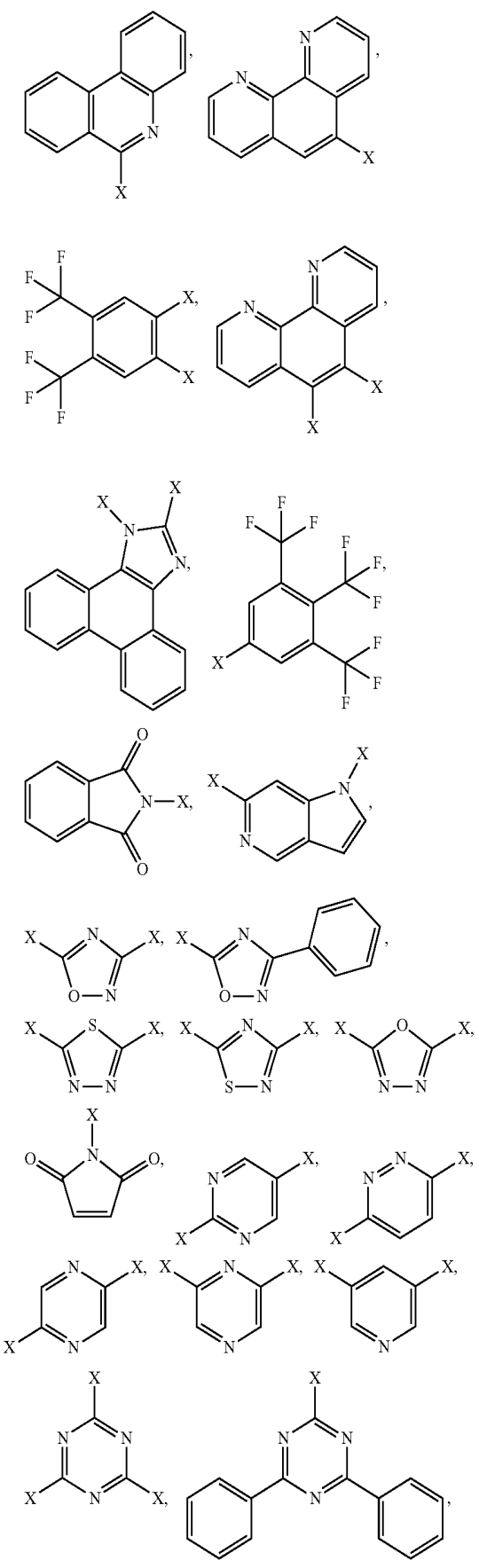

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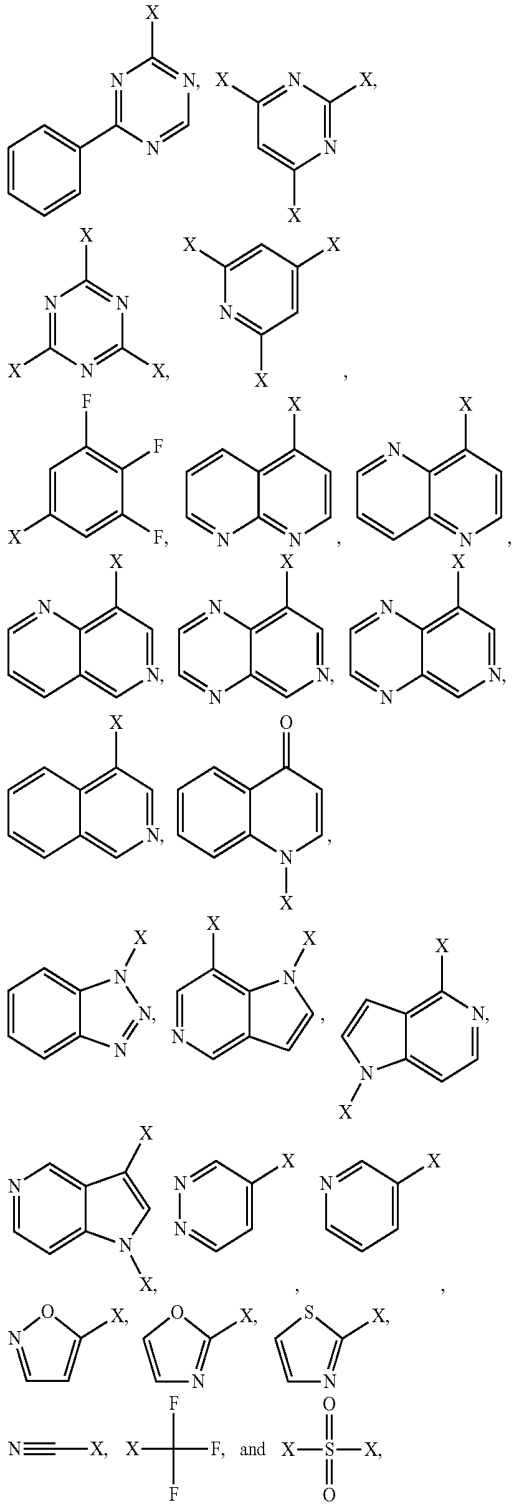


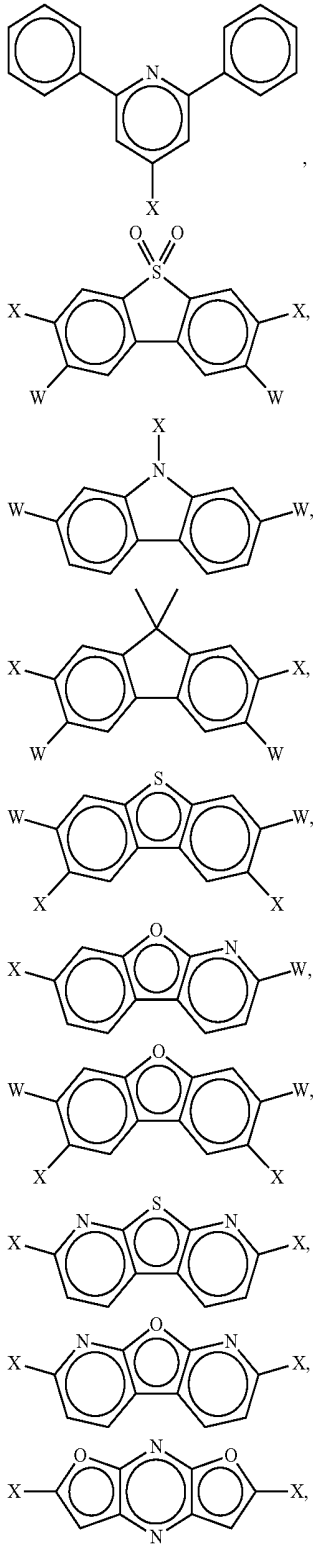
wherein, within each molecule:

[0127] X is selected from the group consisting of the moiety D, a moiety B_{0-2}-D, H, C_1-C_3 alkyl, C_6-C_{18} aryl , oxo, C_1-C_3 haloalkyl, —CN, —CF_3, —$C(O)C_1$-C_3 haloalkyl, —F, and —$S(O_2)H$, and wherein the moieties D and B are defined above with respect to the first, second, and third aspects of the present invention.

[0128] In an example embodiment of the tenth and eleventh aspects of the present invention, the moiety A, for each occurrence independently, can be selected from List A4, List A5, List A6, or any combination thereof.

List A6

[0129]



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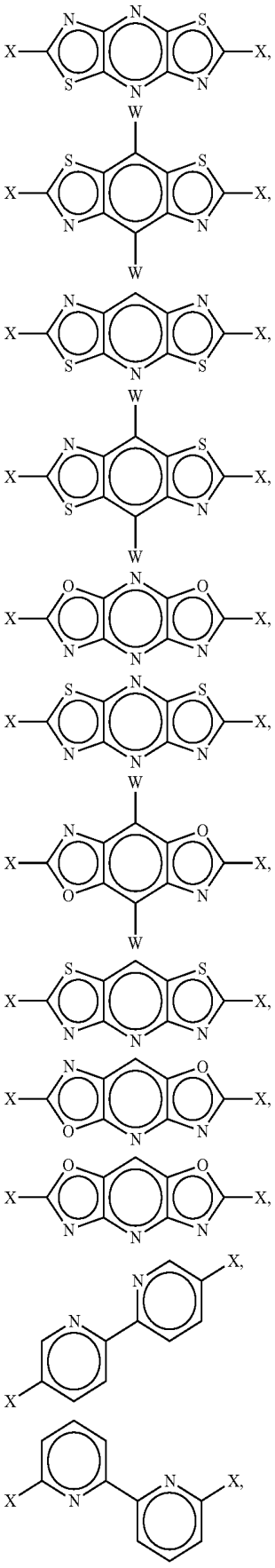

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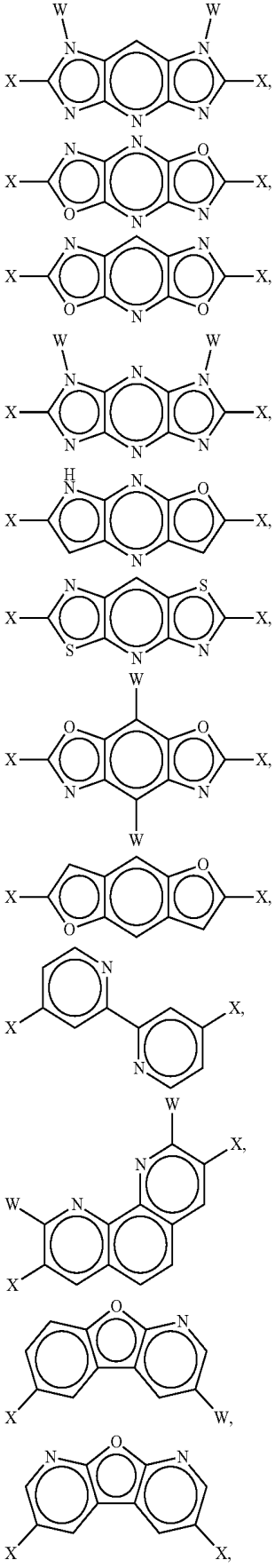

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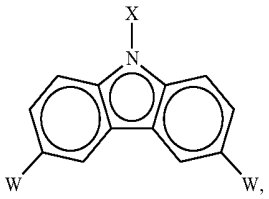

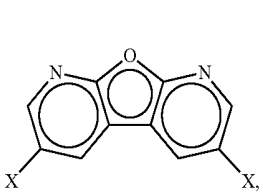

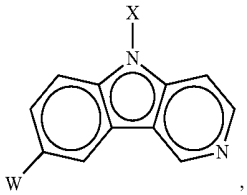

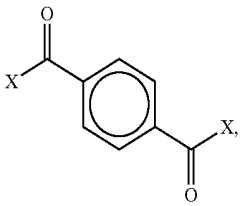

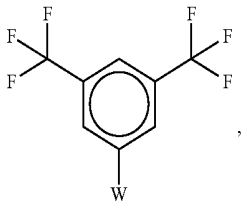

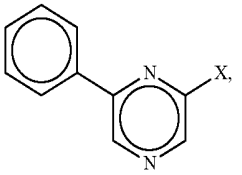

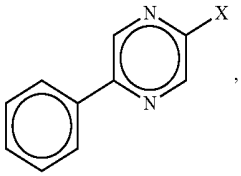

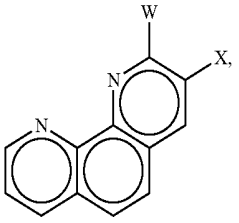

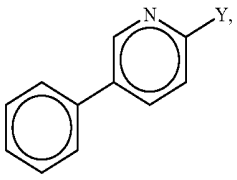

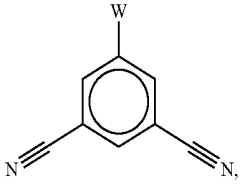

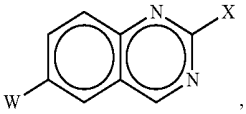

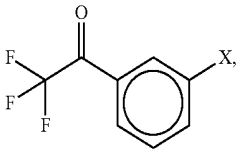

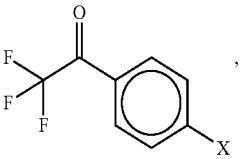

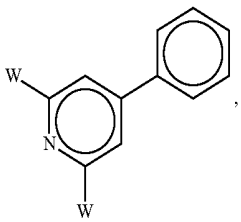

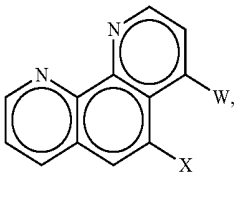

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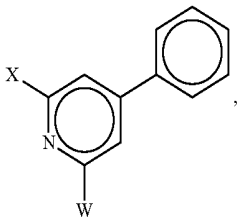

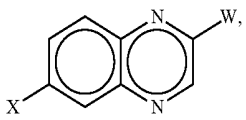

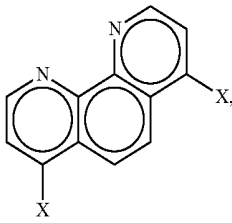

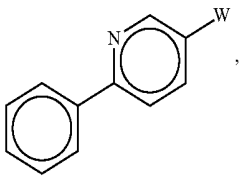

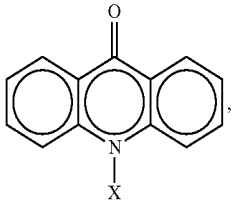

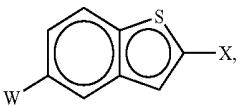

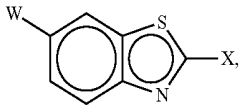

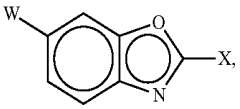

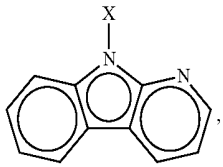

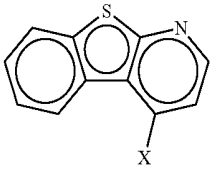

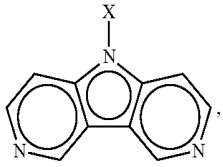

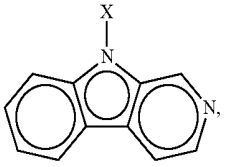

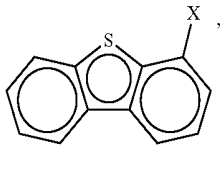

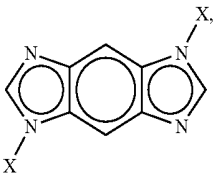

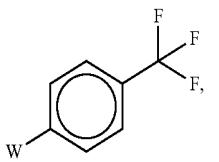

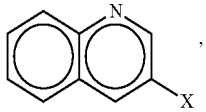

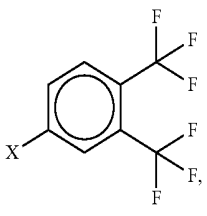

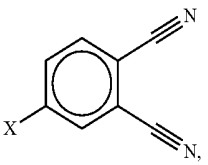

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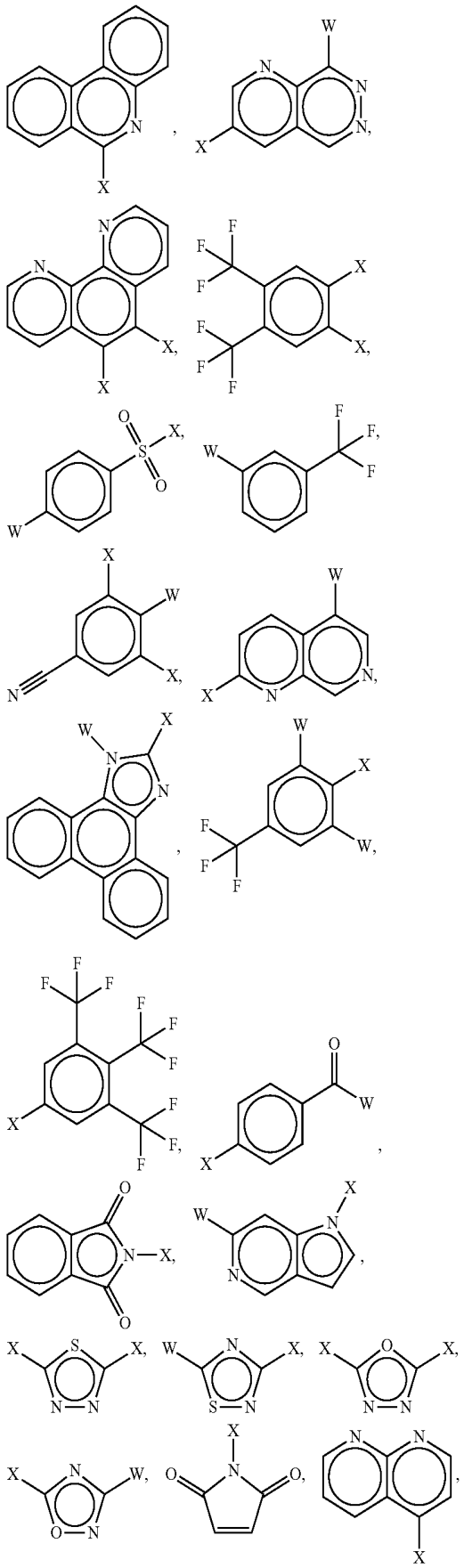

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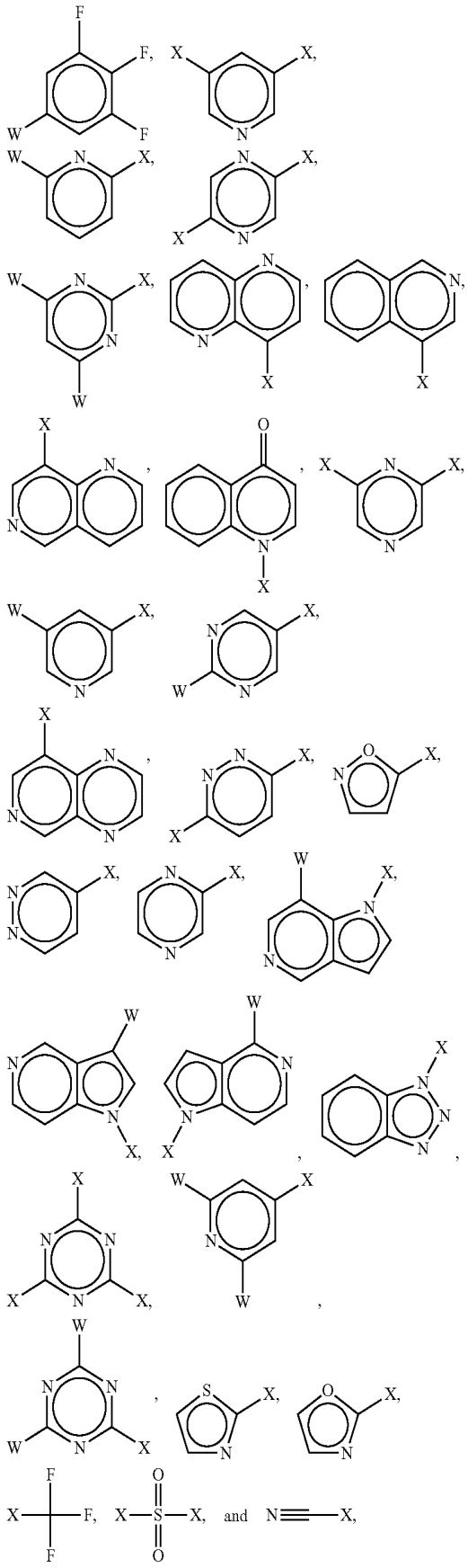


wherein, within each molecule:

[0130] X is selected from the group consisting of a moiety B_{0-2}-D, H, C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, C_1-C_3 haloalkyl, —CN, —CF_3, —C(O)C_1-C_3 haloalkyl, —F, and —$S(O_2)$H,

[0131] W is selected from the group consisting of the moiety B_{0-2}-D, H, C_1-C_3 alkyl, C_1-C_3 acylalkyl, C_6-C_{18} aryl, oxo, C_1-C_3 haloalkyl, —CN, —CF_3, —C(O)C_1-C_3 haloalkyl, —F, and —$S(O_2)$H,

[0132] at least one of W and X is the moiety B_{0-2}-D,

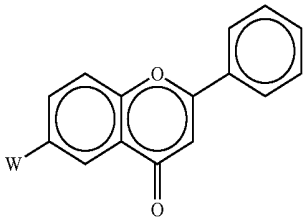
[0133] all groups W are the same and all groups X are the same, and

[0134] each group W is the same or different from any group X, and wherein the moieties D and B are defined above with respect to the first, second, and third aspects of the present invention.

[0135] In an example embodiment of the tenth and eleventh aspects of the present invention, the moiety A, for each occurrence independently, can be selected from List A4, List A5, List A6, List AN2, or any combination thereof. In certain embodiments, at least one occurrence of the moiety A is selected from List AN2. In certain embodiments, each occurrence of the moiety A is independently selected from List AN2.

List AN2

[0136]



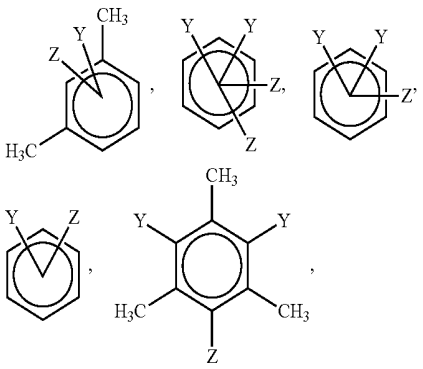
wherein, within each molecule:

[0137] W is the moiety D or a moiety B_{0-2}-D and wherein the moieties D and B are defined above with respect to the first, second, and third aspects of the present invention.

[0138] In an example embodiment of the twelfth aspect of the present invention, the moiety B, for each occurrence independently, is selected from List B3.

List B3

[0139]



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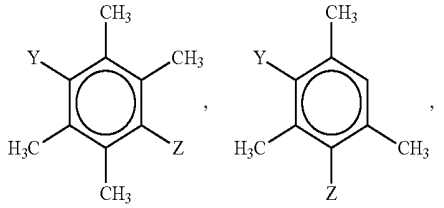


wherein, within each molecule:

[0140] Y is the moiety A, the moiety B_{0-1}-A, the moiety D, or the moiety B_{0-1}-D and each Z is the moiety A, a moiety B_{0-1}-A, the moiety D, or a moiety B_{0-1}-D,

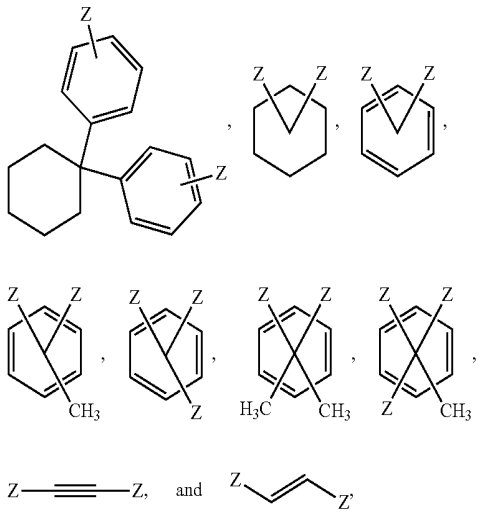
[0141] within a given molecule all groups Y are the same and all groups Z are the same, and

[0142] each group Y is the same or different from any group Z, and wherein the moieties A and D are defined above with respect to the first, second, and third aspects of the present invention.

[0143] In an example embodiment of the thirteenth aspect of the present invention, the moiety B, can also be selected from List B3, List B4, or both.

List B4

[0144]



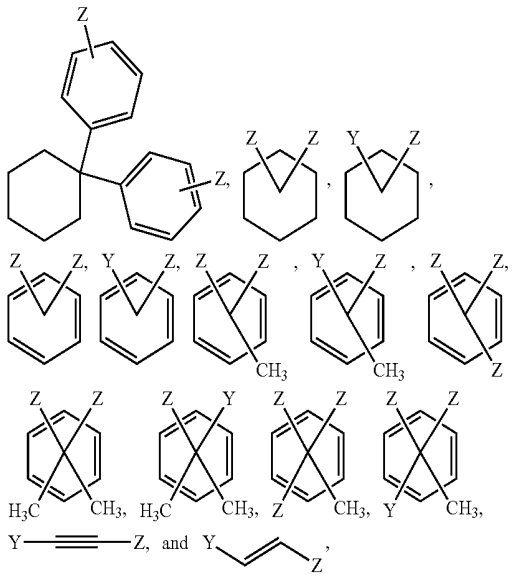
wherein, within each molecule:

[0145] Z is independently selected from the group consisting of the moiety A, a moiety B_{0-1}-A, the moiety D, a moiety B_{0-1}-D, H, C_1-C_3 alkyl, and C_6-C_{18} aryl, and wherein the moieties A and D are defined above with respect to the first, second, and third aspects of the present invention.

[0146] In an example embodiment of the twelfth and thirteenth aspects of the present invention, the moiety B, can also be selected from List B3, List B4, List B5, or any combination thereof.

List B5

[0147]



wherein, within each molecule:

[0148] Z is the moiety A, a moiety B_{0-1}-A, the moiety D, a moiety B_{0-1}-D, H, C_1-C_3 alkyl, or C_6-C_{18} aryl,

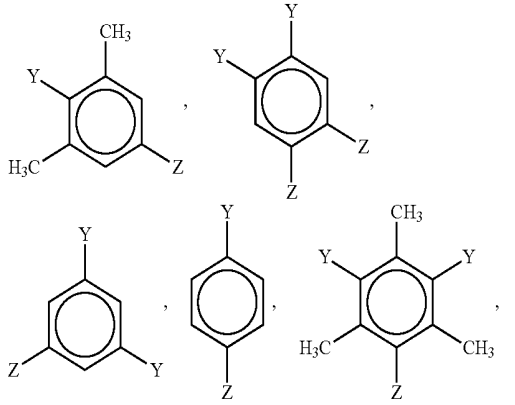
[0149] Y is the moiety A, the moiety B_{0-1}-A, the moiety D, or the moiety B_{0-1}-D and each Z is the moiety A, a moiety B_{0-1}-A, the moiety D, or a moiety B_{0-1}-D,

[0150] within a given molecule all groups Y are the same and all groups Z are the same, and

[0151] each group Y is the same or different from any group Z, and wherein the moieties A and D are defined above with respect to the first, second, and third aspects of the present invention.

[0152] In an example embodiment of the twelfth aspect of the present invention, the moiety B, for each occurrence independently, is selected from List B3, List B4, List B5, List B6, or any combination thereof.

[0153] List B6



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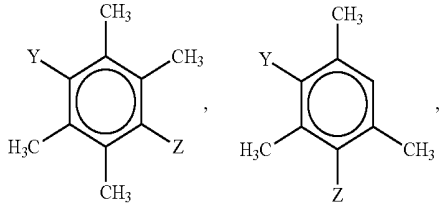


wherein, within each molecule:

[0154] Y is the moiety A, the moiety B_{0-1}-A, the moiety D, or the moiety B_{0-1}-D and each Z is the moiety A, a moiety B_{0-1}-A, the moiety D, or a moiety B_{0-1}-D,

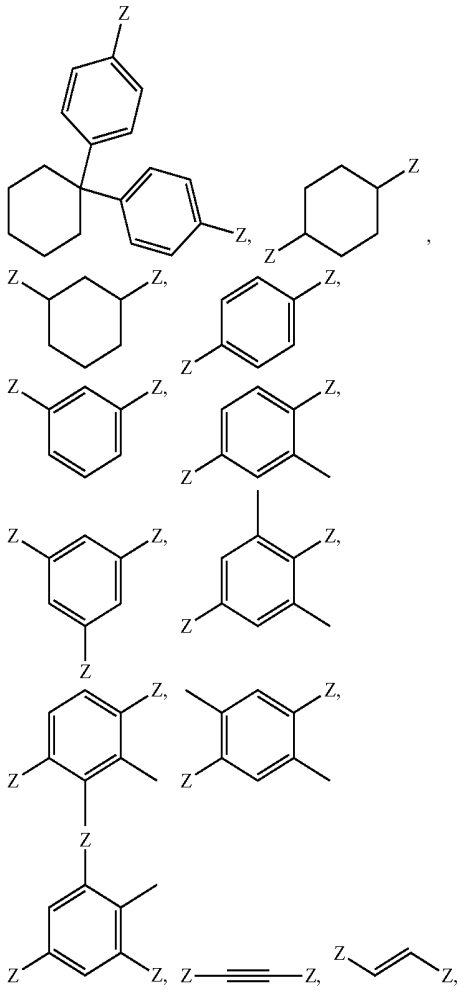
[0155] within a given molecule all groups Y are the same and all groups Z are the same, and

[0156] each group Y is the same or different from any group Z, and wherein the moieties A and D are defined above with respect to the first, second, and third aspects of the present invention.

[0157] In an example embodiment of the thirteenth aspect of the present invention, the moiety B, for each occurrence independently, is selected from List B3, List B4, List B5, List B6, List B7, or any combination thereof.

List B7

[0158]



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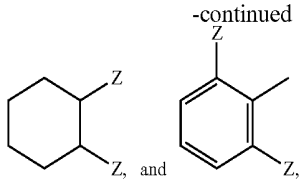


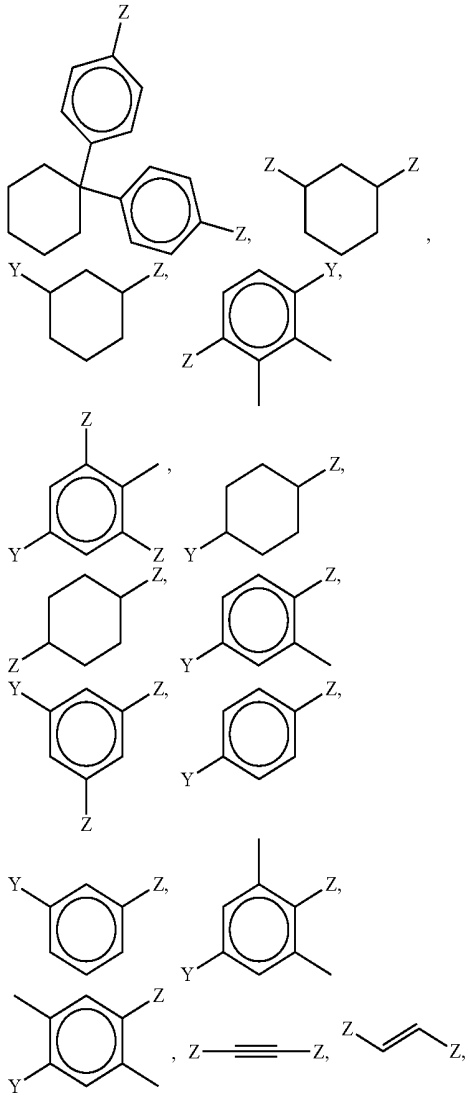
wherein, within each molecule:

[0159] Z is the moiety A, the moiety B_{0-1}-A, the moiety D, the moiety B_{0-1}-D, H, C_1-C_3 alkyl, or C_6-C_{18} aryl, and wherein the moieties A and D are defined above with respect to the first, second, and third aspects of the present invention.

[0160] In an example embodiment of the twelfth and thirteenth aspects of the present invention, the moiety B, for each occurrence independently, is selected from List B3, List B4, List B5, List B6, List B7, List B8 or any combination thereof.

List B8

[0161]



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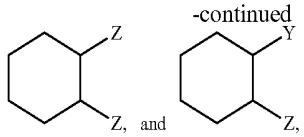


wherein, within each molecule:

[0162] Z is the moiety A, the moiety B_{0-1}-A, the moiety D, the moiety B_{0-1}-D, H, C_1-C_3 alkyl, or C_6-C_{18} aryl,

[0163] Y is the moiety A, the moiety B_{0-1}-A, the moiety D, the moiety B_{0-1}-D, H, C_1-C_3 alkyl, or C_6-C_{18} aryl,

[0164] within a given molecule all groups Y are the same and all groups Z are the same, and

[0165] each group Y is the same or different from any group Z, and wherein the moieties A and D are defined above with respect to the first, second, and third aspects of the present invention.

[0166] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety D is optionally substituted with one or more substituents each independently selected from C_1-C_3 alkyl, C_6-C_{18} aryl, or oxo, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0167] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety D is optionally substituted with one or more substituents each independently selected from (5-20 atom) heteroaryl or —$N(C_6$-$C_{18}aryl)_2$, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0168] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety D is optionally substituted with one or more substituents each independently selected from C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, (5-20 atom) heteroaryl, or —$N(C_6$-$C_{18}aryl)_2$, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0169] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety A is optionally substituted with one or more substituents each independently selected from C_1-C_3 alkyl, C_6-C_{18} aryl, oxo, C_1-C_3 haloalkyl, —CN, —CF_3, —$C(O)C_1$-C_3 haloalkyl, —F, and —$S(O_2)$H, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0170] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety B is optionally substituted with C_1-C_3 alkyl, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0171] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety B is optionally substituted with C_6-C_{18} aryl, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0172] In an example embodiment of any one of the first through thirteenth aspects of the present invention described above, the moiety B is optionally substituted with one or more substituents each independently selected from C_1-C_3 alkyl or C_6-C_{18} aryl, and wherein A, B, and D are defined above with respect to the first or second aspects of the present invention.

[0173] In a fourteenth aspect, the present invention is a molecule of any one of the structural formulas represented in Tables M, N, O, Q, B, or R and is optionally substituted.

[0174] According to certain embodiments of the fourteenth aspect, the present invention is a molecule represented by any one structural formula in Tables M, N, O, Q, B, or R and is optionally substituted. According to certain embodiments, the present invention is a molecule represented by any one structural formula in Tables M, N, O, Q, or R and is optionally substituted. According to certain embodiments, the present invention is a molecule represented by any one structural formula in Tables N', N'', N''', Q', or R' and is optionally substituted. The variables and substitution patterns on the molecule may be selected as described below with respect to the fourteenth aspect.

[0175] According to certain embodiments of the fourteenth aspect, the present invention is a molecule represented by any one structural formula as shown in Table M, N, N', N'', N''', O, Q, Q', B, R, or R', wherein

[0176] at each substitutable carbon independently, the molecule is optionally substituted with R^C;

[0177] R^C is selected from a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, —OH, —CN, a halo, a C_6-C_{12} aryl, a 5-20 atom heteroaryl, or —$N(R^{19})_2$; and

[0178] each R^{19}, independently, is H, a C_1-C_6 alkyl, a C_5-C_{12} cycloalkyl, or a C_6-C_{18} aryl.

[0179] According to certain embodiments of the fourteenth aspect, the molecule is represented by one of the structural formulas in Table M, N, N', N'', N''', O, Q, Q', B, R, or R', and is optionally substituted at any substitutable carbon with R^C. According to certain embodiments, no atom is substituted. According to certain embodiments, at least one substitutable carbon is substituted with R^C. The variables and base molecules may be selected as described above or below with respect to the fourteenth aspect.

[0180] According to certain embodiments of the fourteenth aspect, the molecule is represented by any one compound in Tables M, N, O, Q, B, R, N', N'', N''', Q', or R' wherein atoms marked with * are optionally substituted with R^C. According to certain embodiments, no atom is substituted with R^C. According to certain embodiments, at least one atom marked with * is substituted with R^C. According to certain embodiments, at least one atom marked with * is substituted with R^C, and any substitutable carbon is optionally substituted with R^C. According to certain embodiments, at least one atom marked with * is substituted with R^C, and no other atom is substituted. The variables and base molecules may be selected as described above or below with respect to the fourteenth aspect.

[0181] According to certain embodiments of the fourteenth aspect, each R^C, independently, is selected from a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, —OH, —CN, a halo, a C_6-C_{12} aryl, a 5-20 atom heteroaryl, or —$N(R^{19})_2$. According to certain embodiments, each R^C, independently, is selected from a C_1-C_3 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{10} aryl, a 5-20 atom heteroaryl, halo, or —CN. According to certain embodiments of the fourteenth aspect, each R^C, independently, is selected from methyl or phenyl. The remainder of the variables, base molecules, and substitution patterns, may be selected as described above or below with respect to the fourteenth aspect.

[0182] According to example embodiments of the fourteenth aspect, each R^{19}, independently, is H, a C_1-C_6 alkyl, a C_5-C_{12} cycloalkyl, or a C_6-C_{18} aryl. According to certain embodiments, each R^{19}, independently, is H, a C_1-C_3 alkyl, a C_3-C_6 cycloalkyl, or phenyl. According to certain embodiments, each R^{19} is phenyl. The remainder of the variables, base molecules, and substitution patterns, may be selected as described above or below with respect to the fourteenth aspect.

[0183] In an example embodiment of the fourteenth aspect, the present invention is any one molecule selected from compounds M1 to M53, listed in Table M. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE M

M1

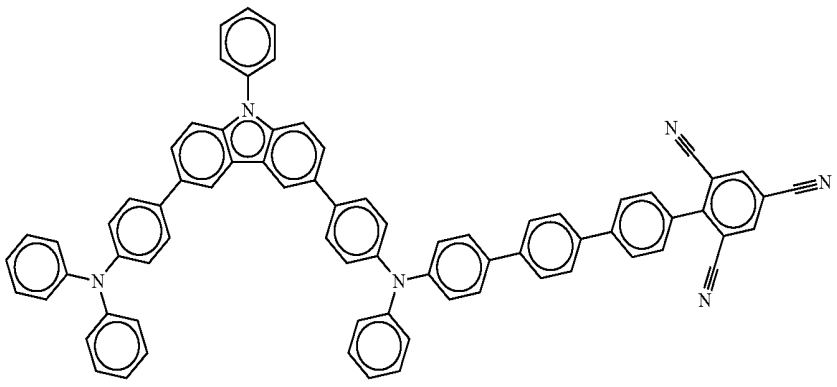
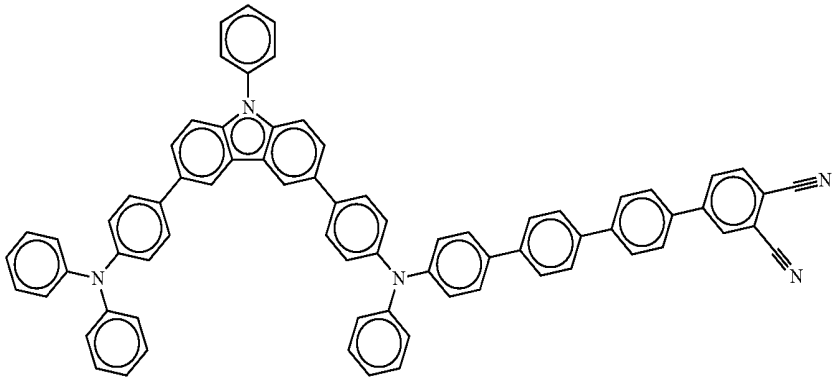
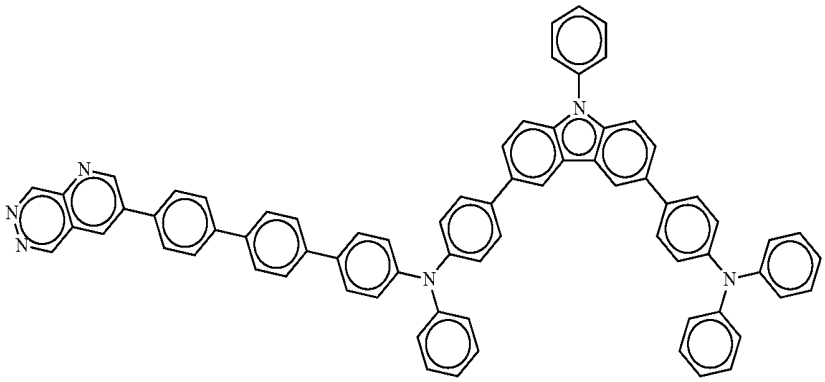


TABLE M-continued

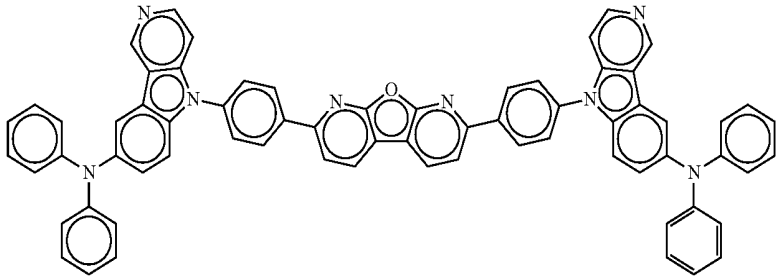
M2



M3



M4



M5

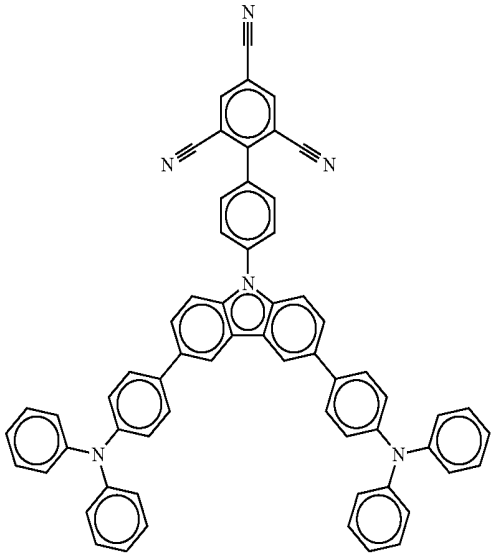
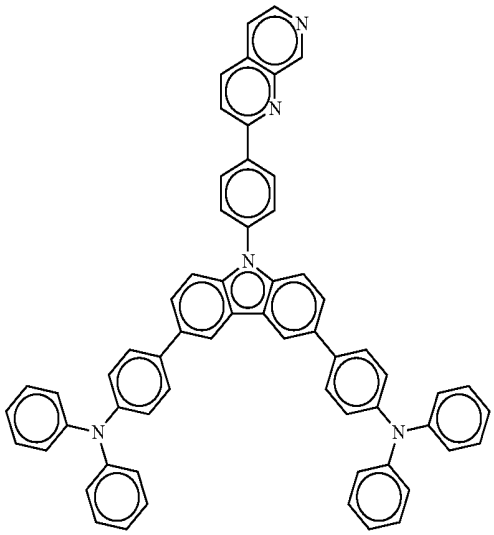


TABLE M-continued

M6



M7

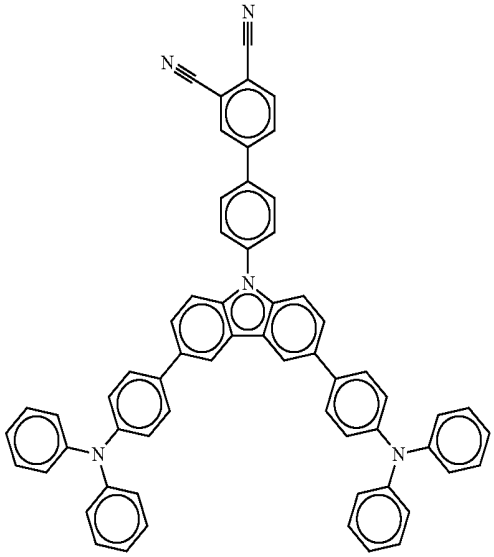
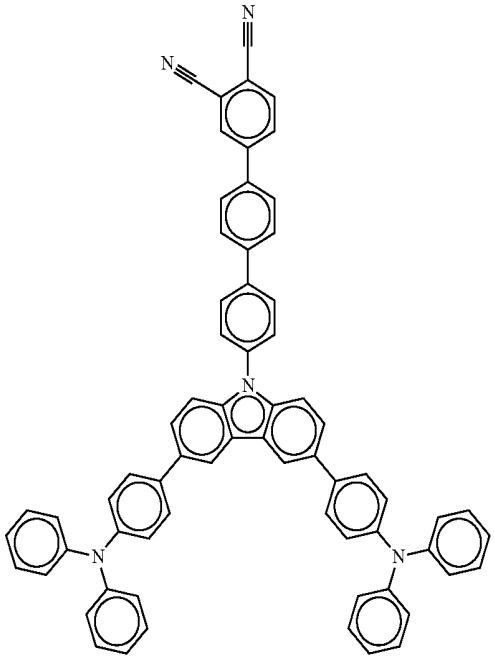


TABLE M-continued

M8



M9

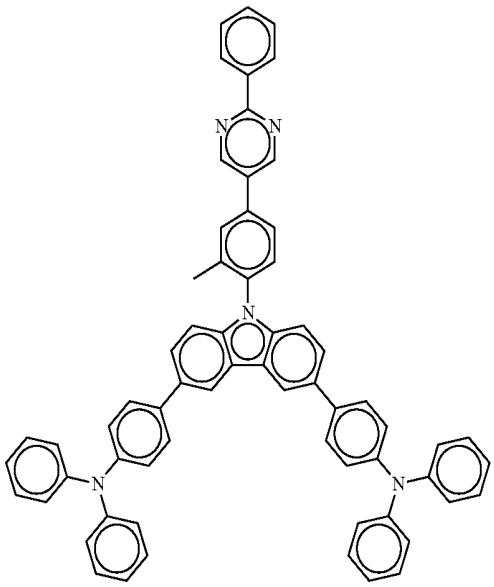
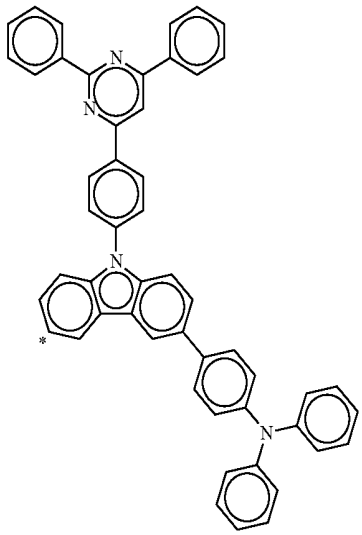


TABLE M-continued

M10



M11

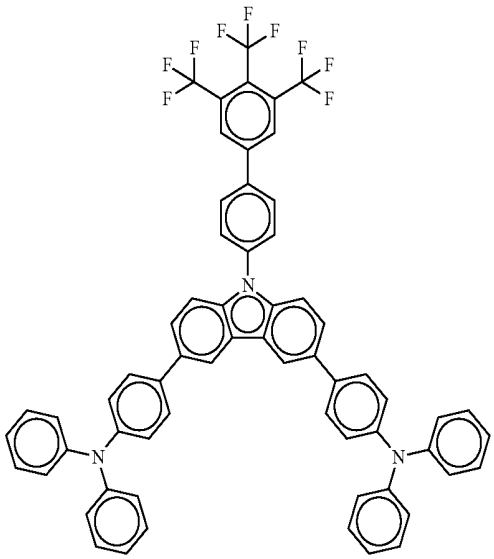
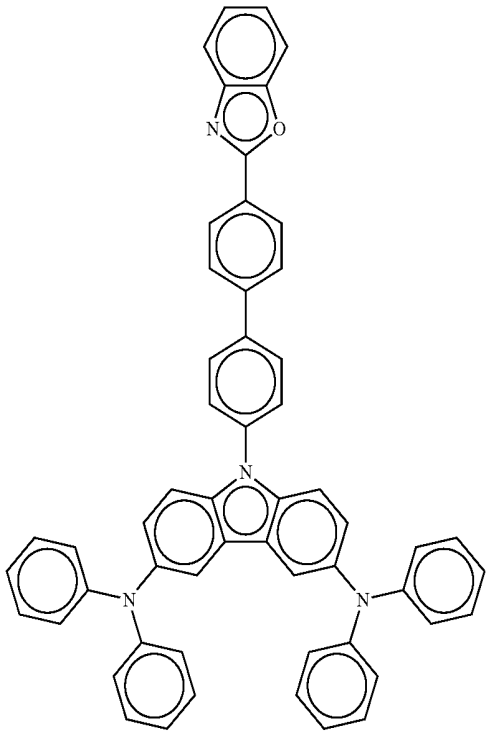


TABLE M-continued

M12



M13

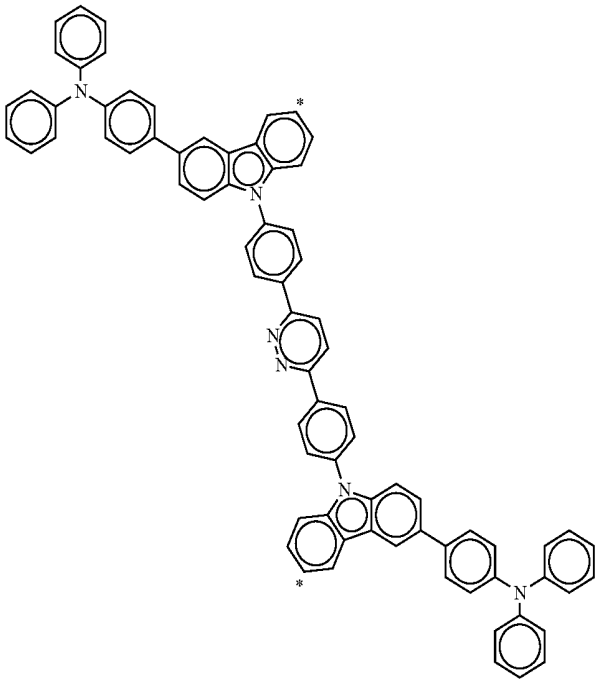
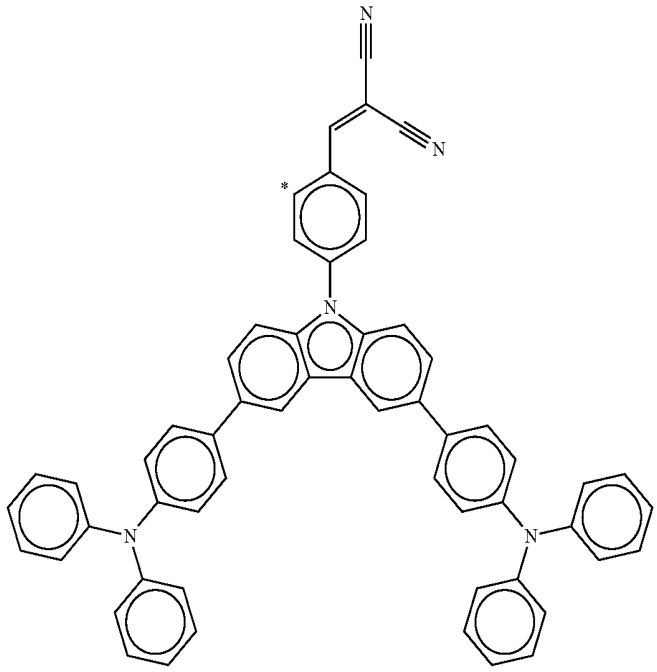


TABLE M-continued

M14



M15

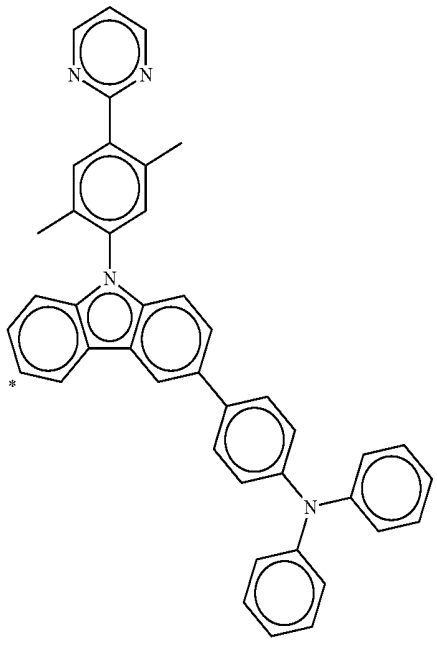
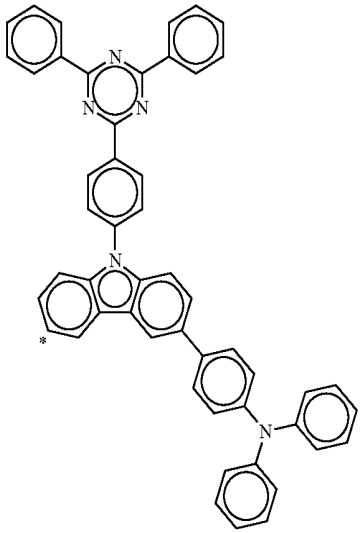


TABLE M-continued

M16



M17

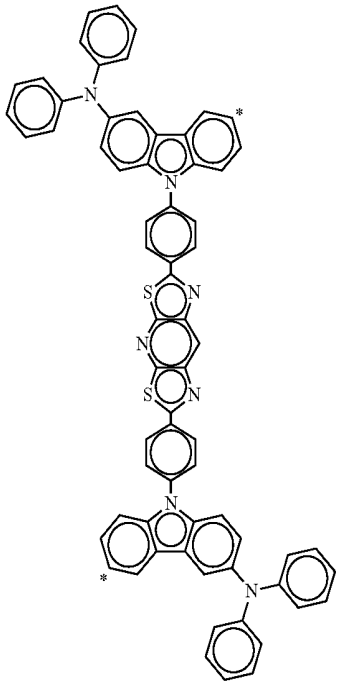
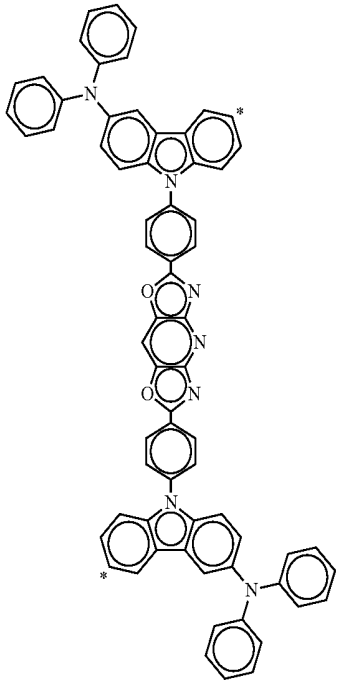


TABLE M-continued

M18



M19

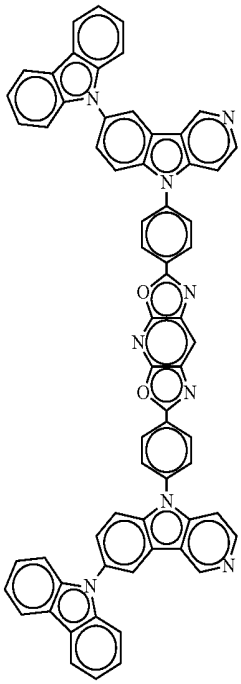
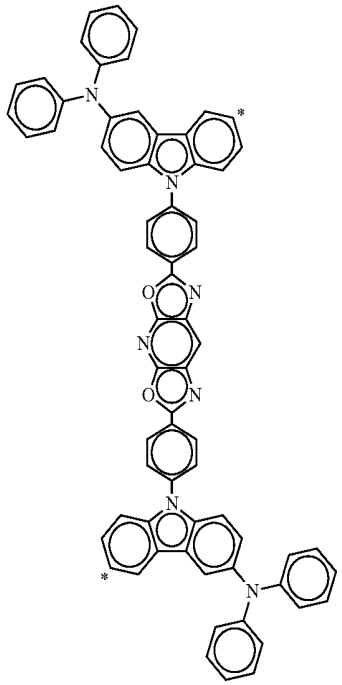
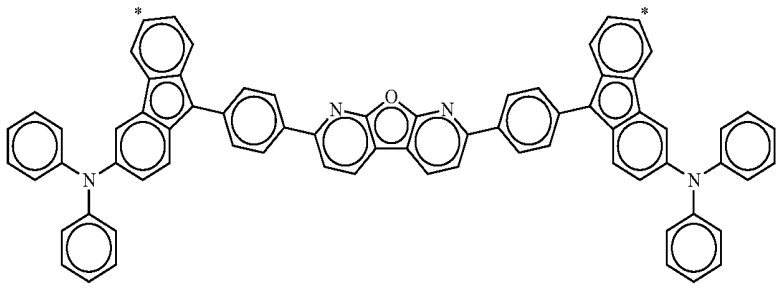


TABLE M-continued

M20



M21



M22

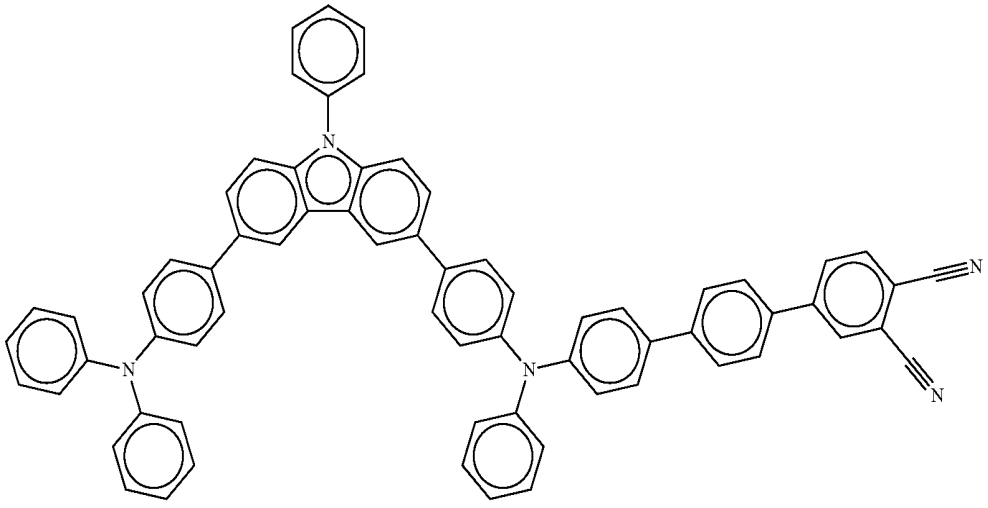
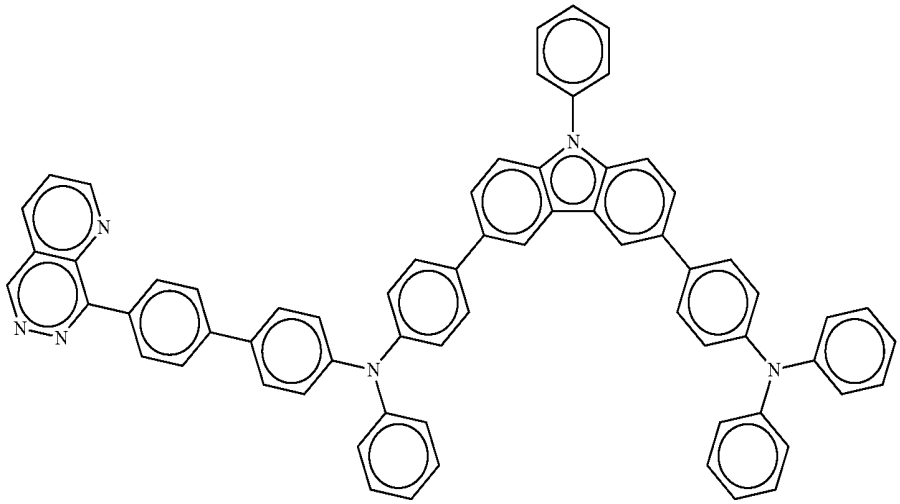
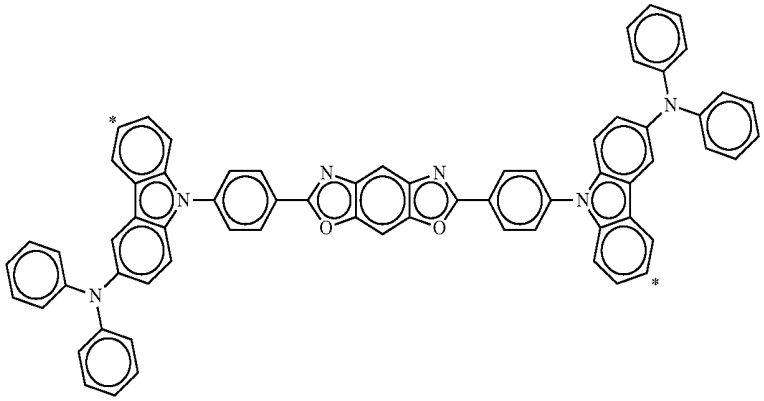


TABLE M-continued

M23



M24



M25

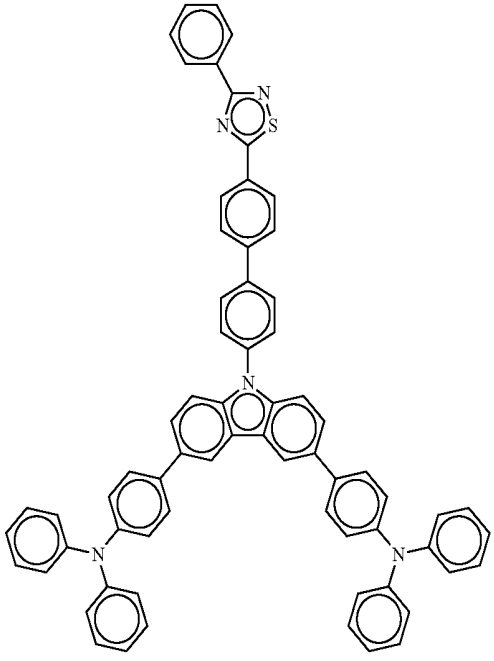
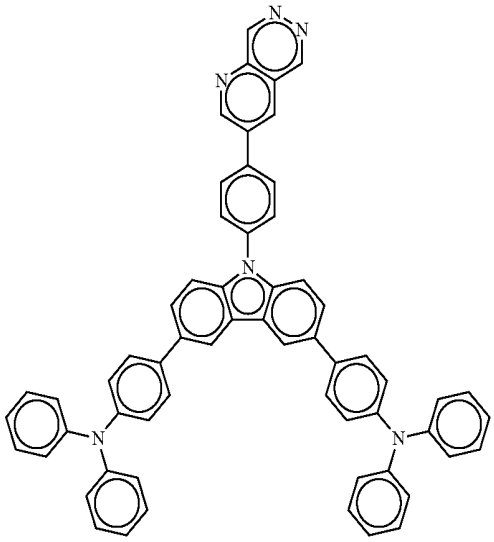
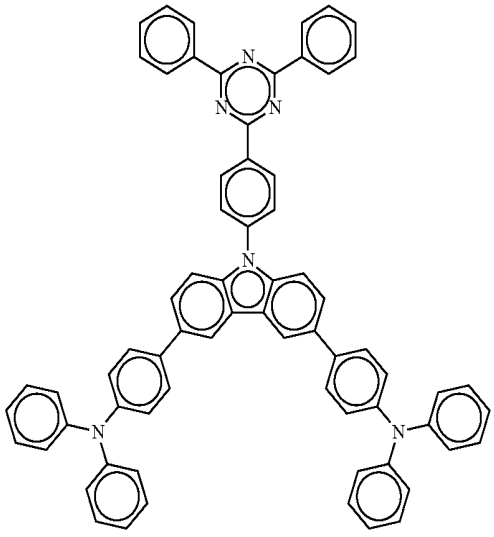


TABLE M-continued

M26



M27



M28

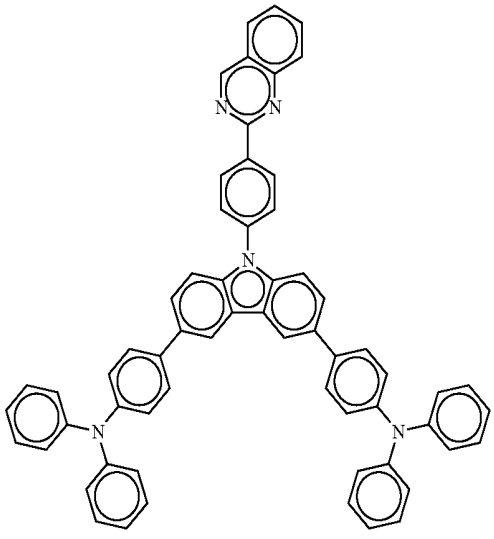
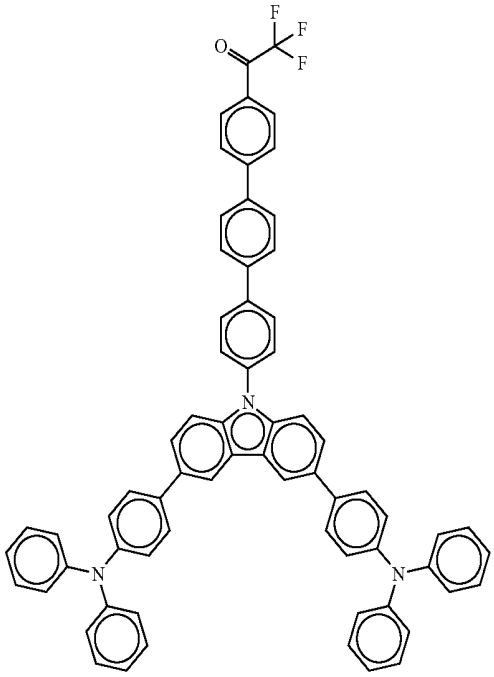


TABLE M-continued

M29



M30

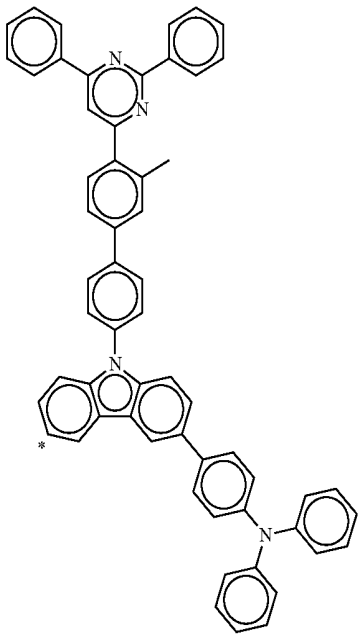
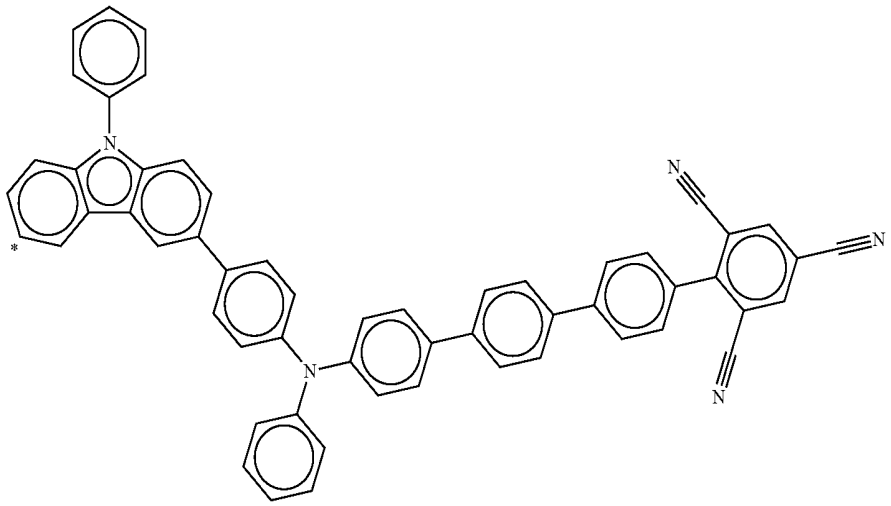


TABLE M-continued

M31



M32

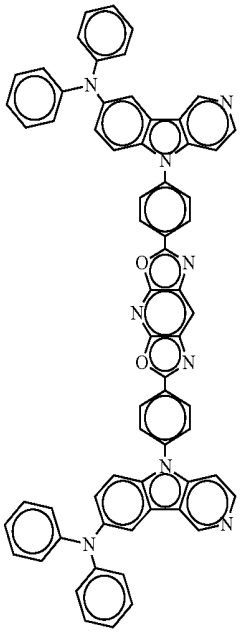
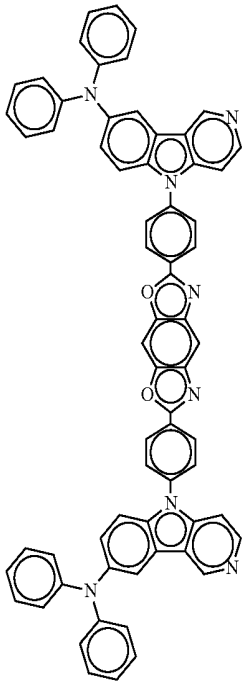


TABLE M-continued

M33



M34

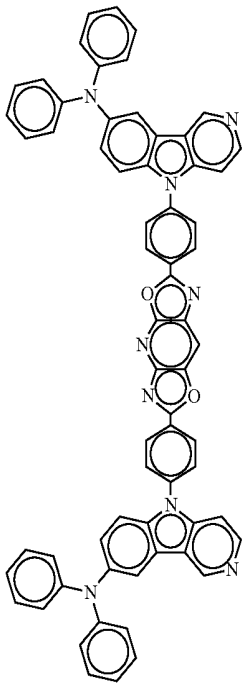
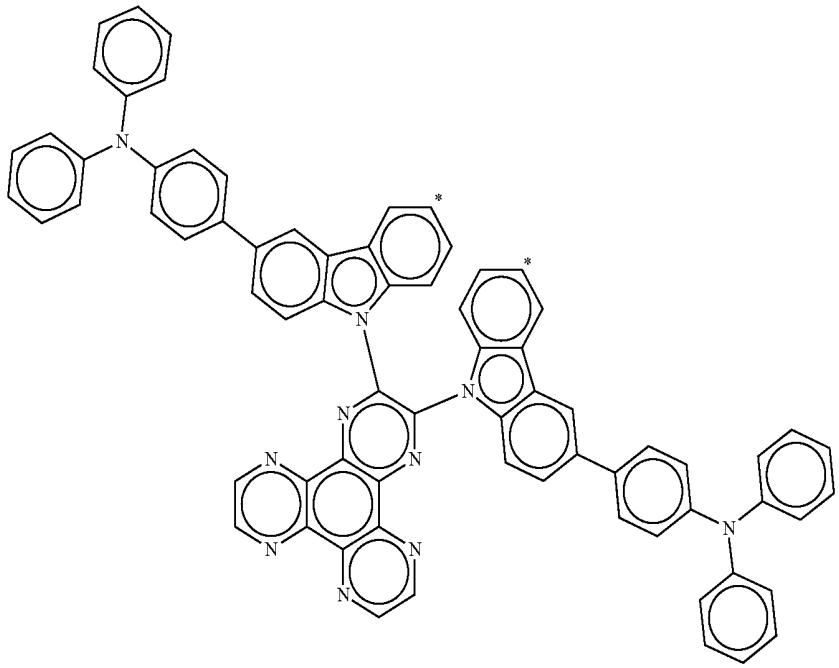
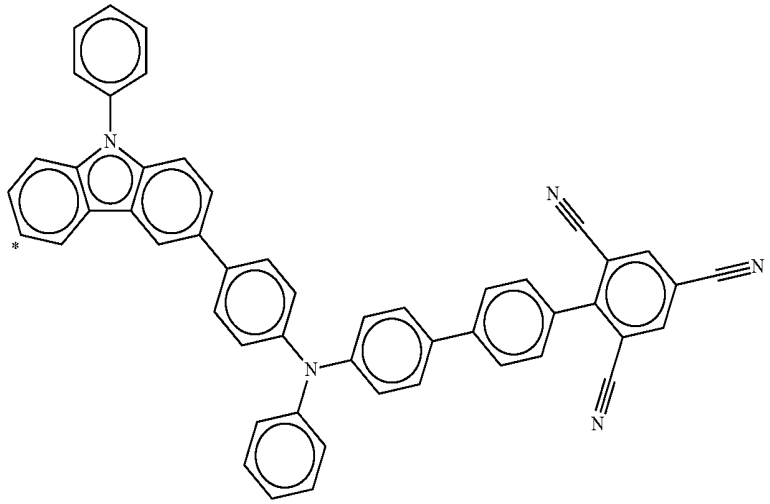


TABLE M-continued

M35



M36



M37

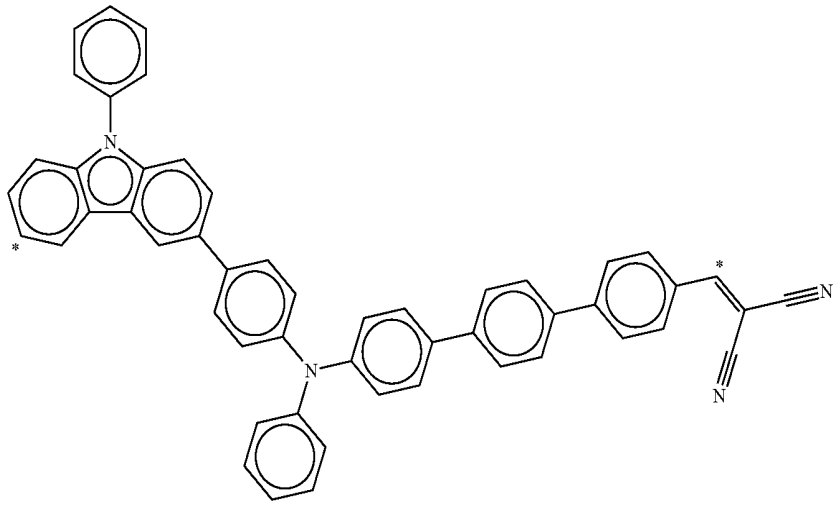
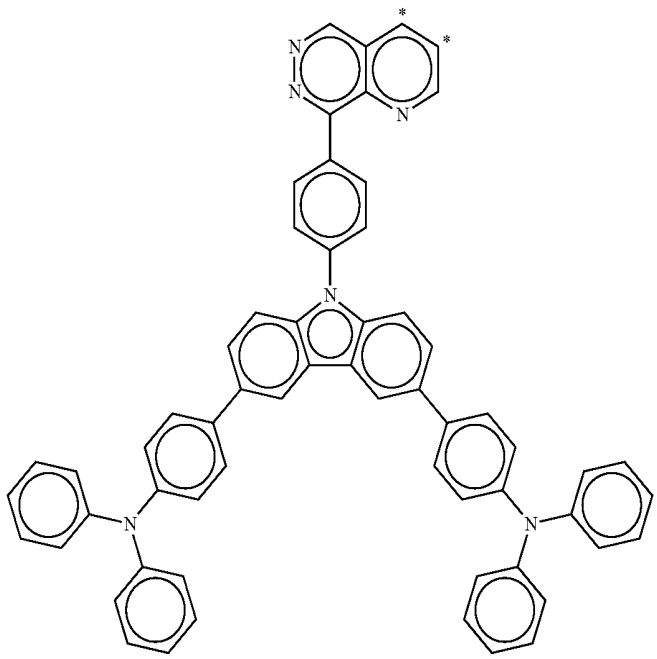


TABLE M-continued

M38



M39

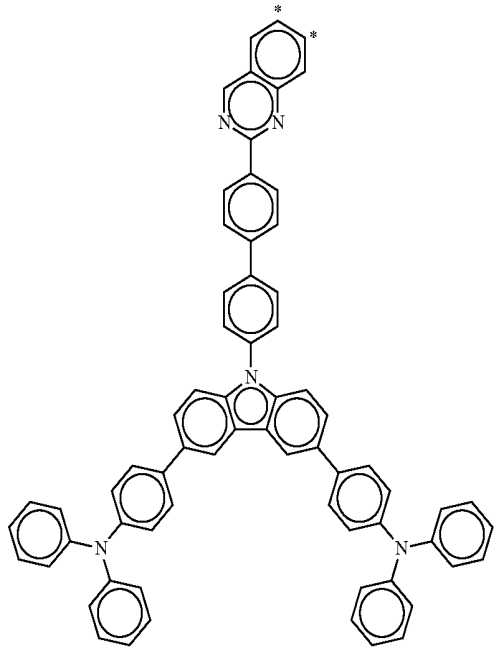
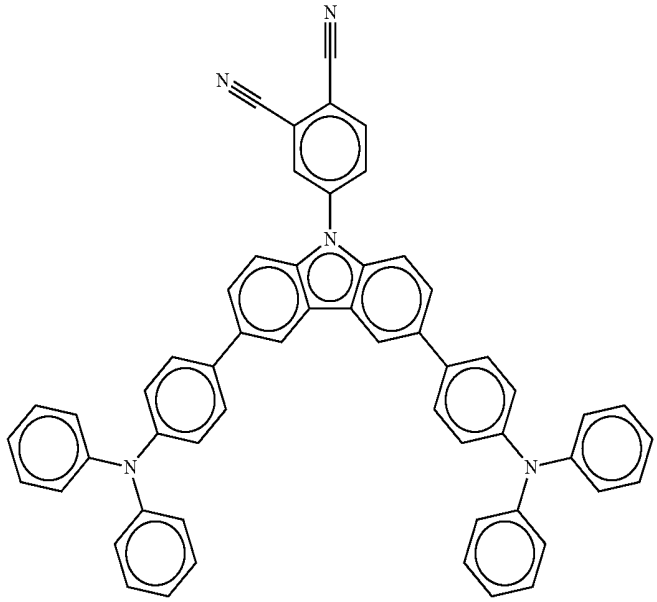
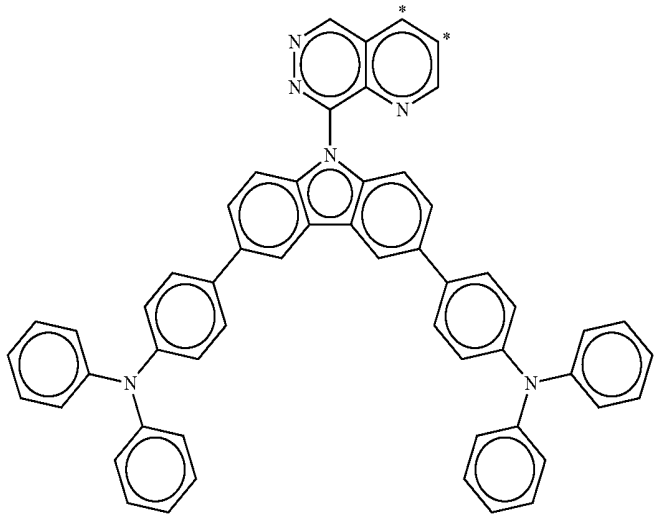


TABLE M-continued

M40



M41



M42

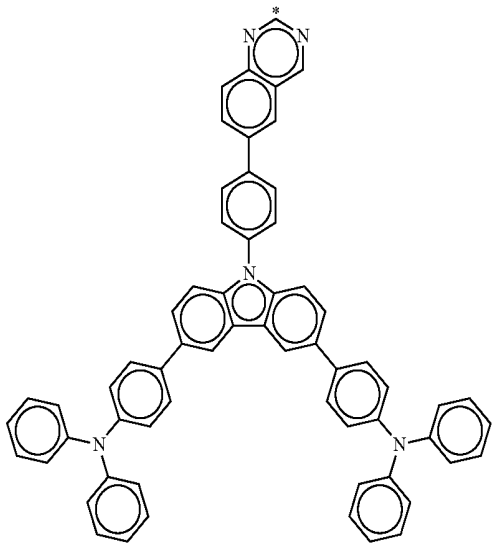
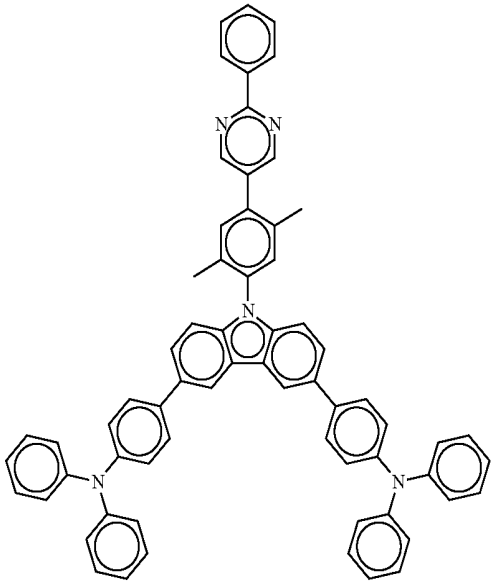


TABLE M-continued

M43



M44

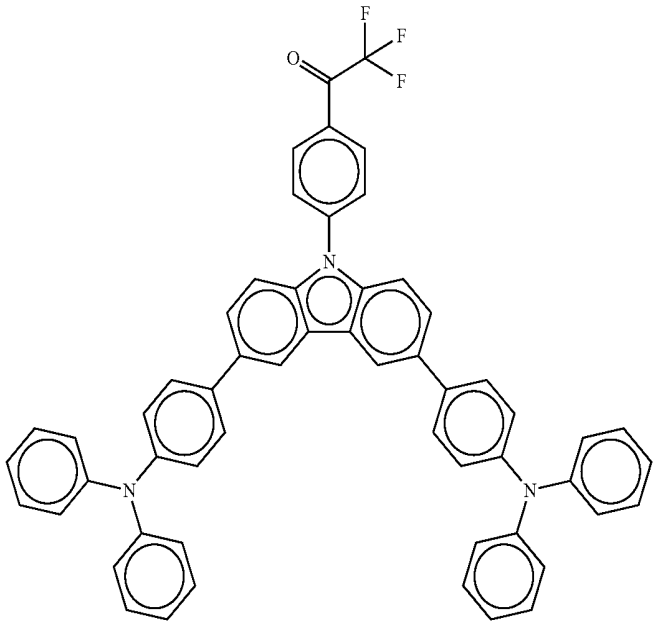
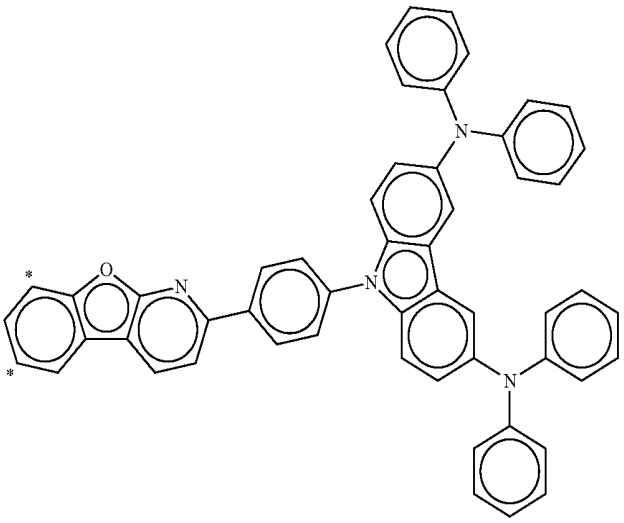
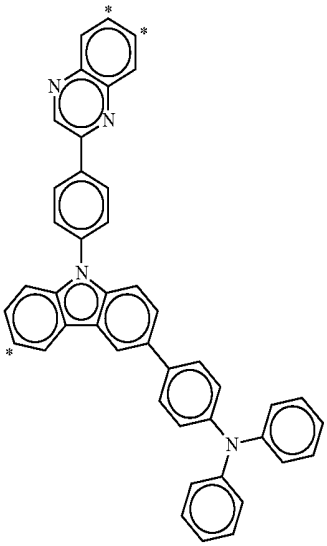


TABLE M-continued

M45



M46



M47

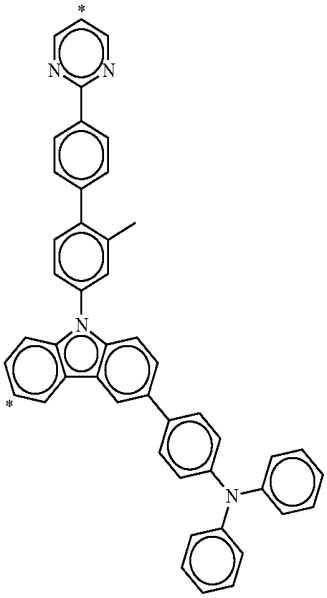
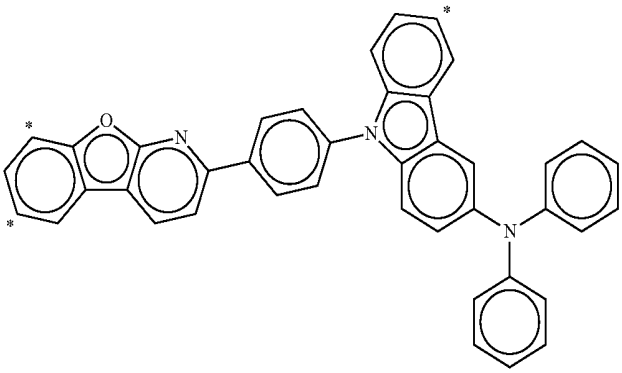
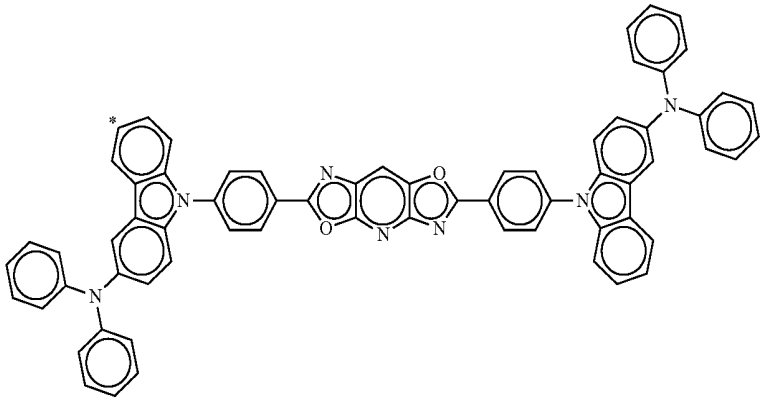


TABLE M-continued

M48



M49



M50

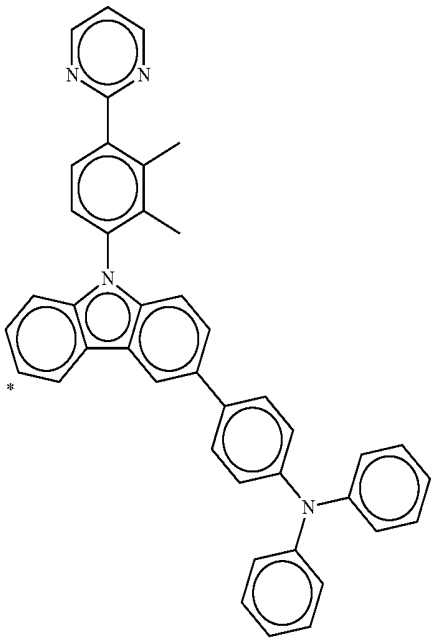
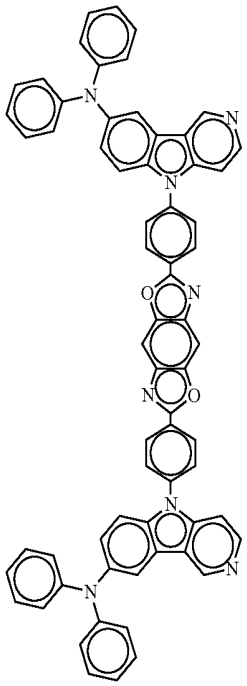


TABLE M-continued

M51



M52

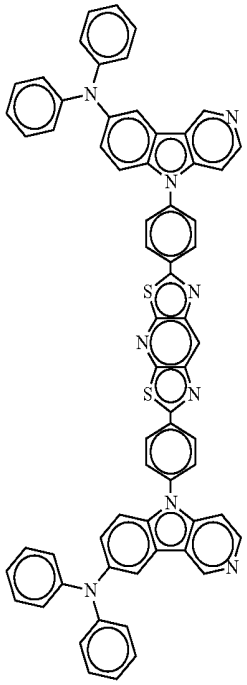
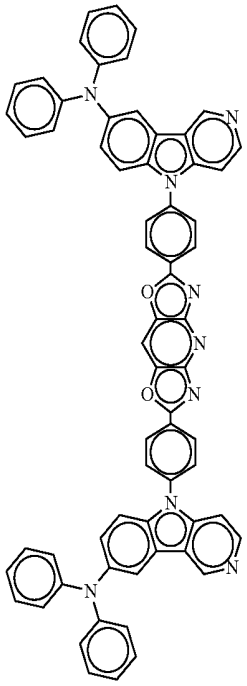


TABLE M-continued

M53



[0184] In an example embodiment of the fourteenth aspect, the present invention is any one molecule selected from compounds N1 to N151, listed in Table N. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE N

N1

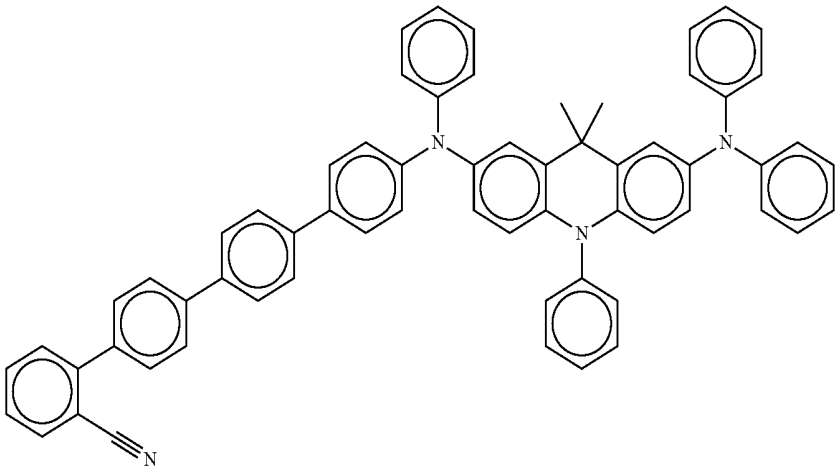
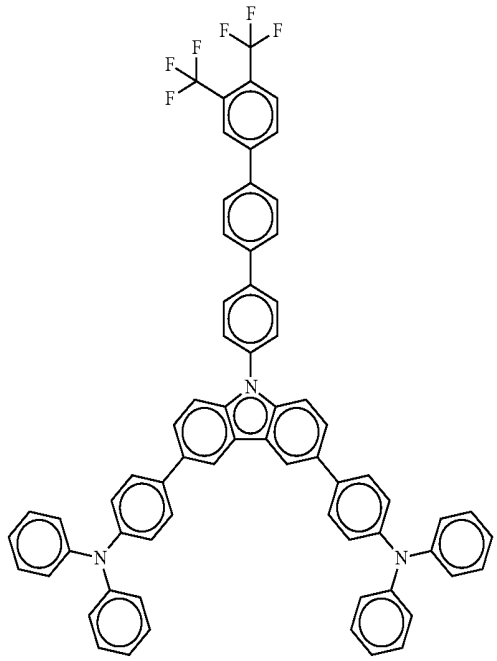


TABLE N-continued

N2



N3

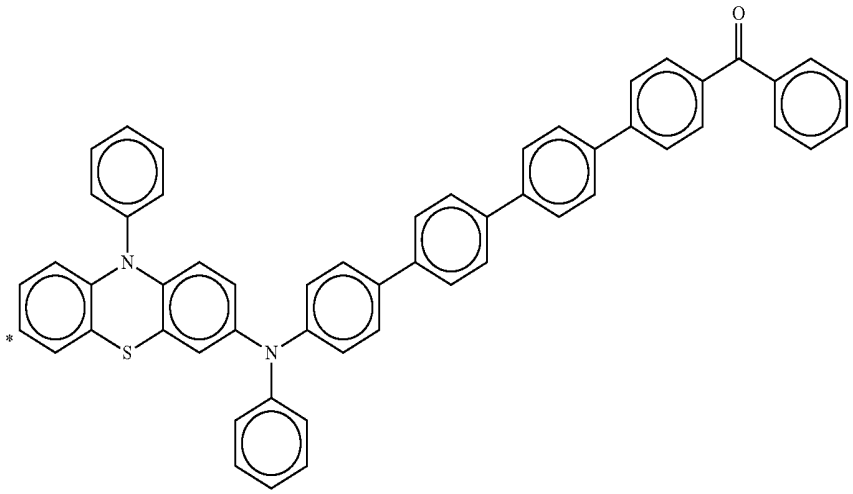
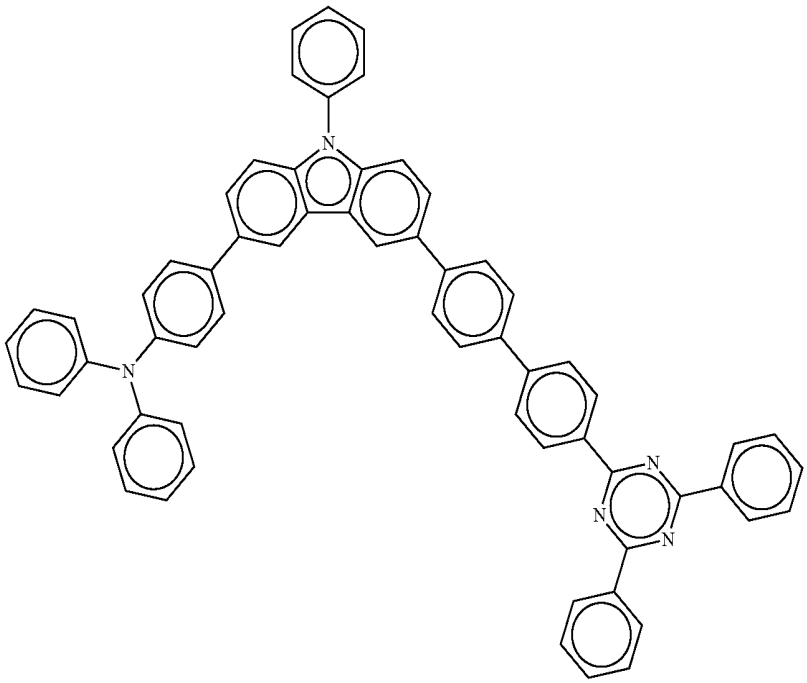


TABLE N-continued

N4



N5

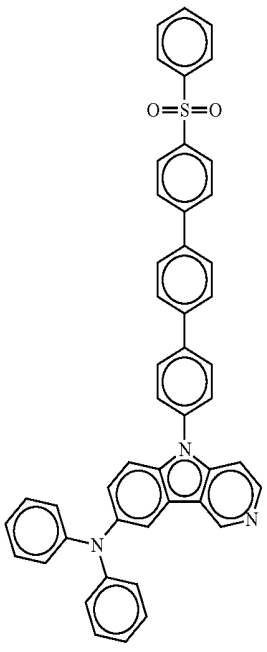
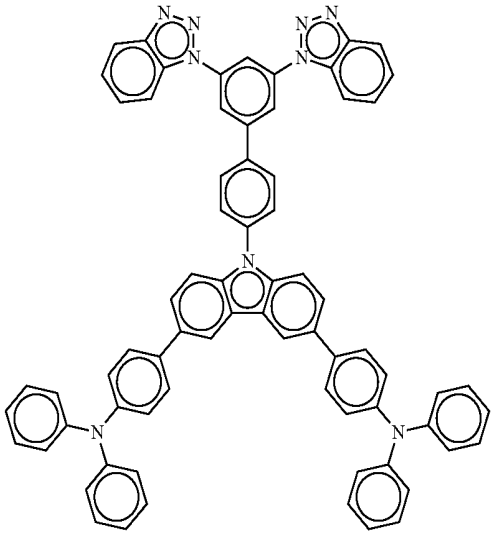


TABLE N-continued

N6



N7

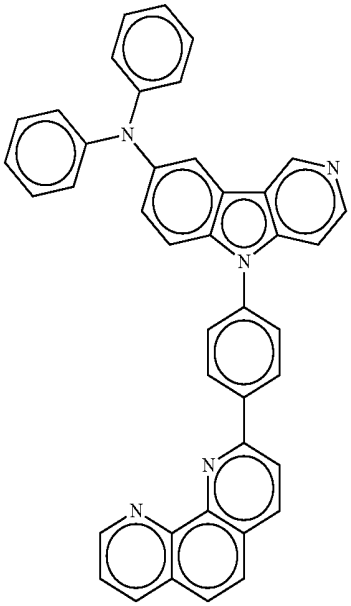
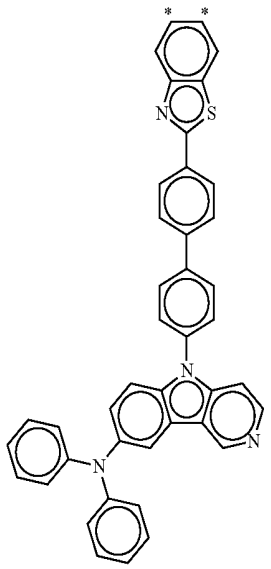


TABLE N-continued

N8



N9

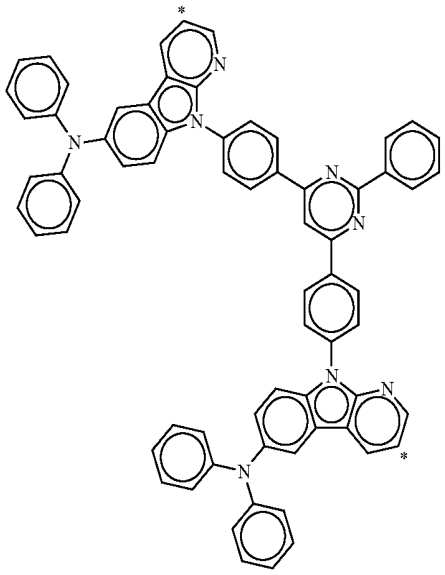
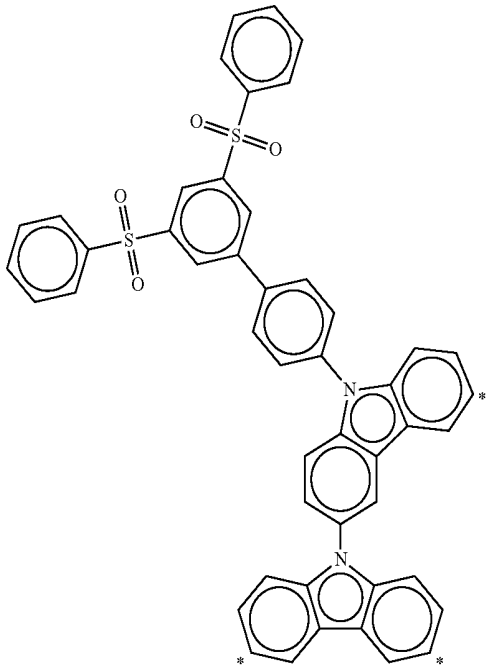


TABLE N-continued

N10



N11

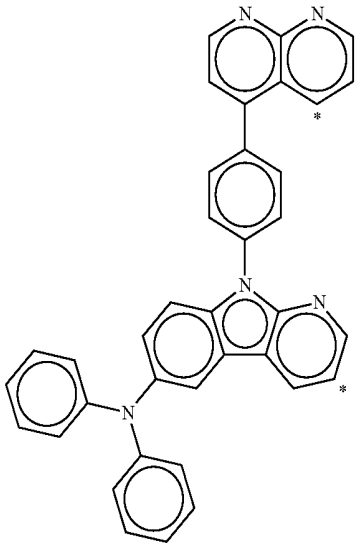
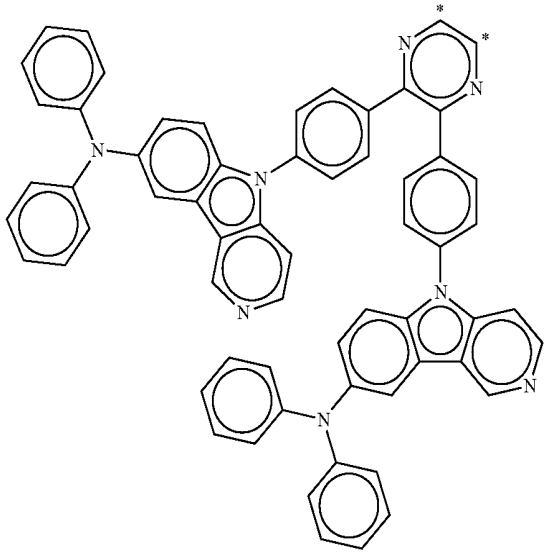
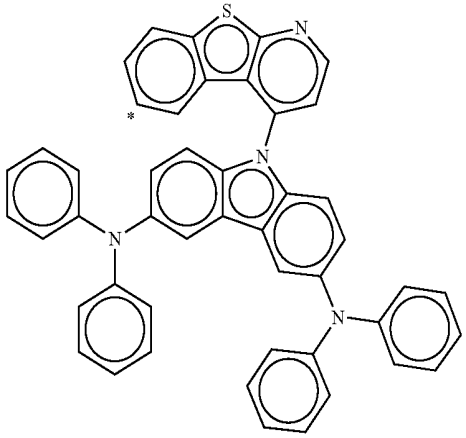


TABLE N-continued

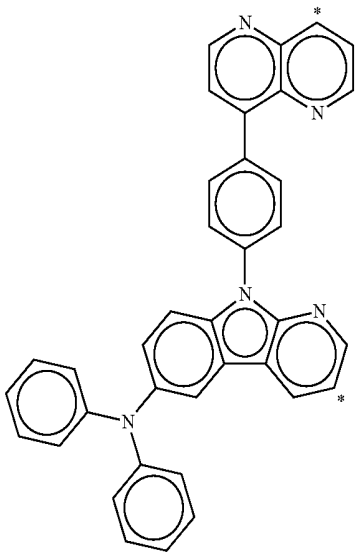
N12



N13



N14



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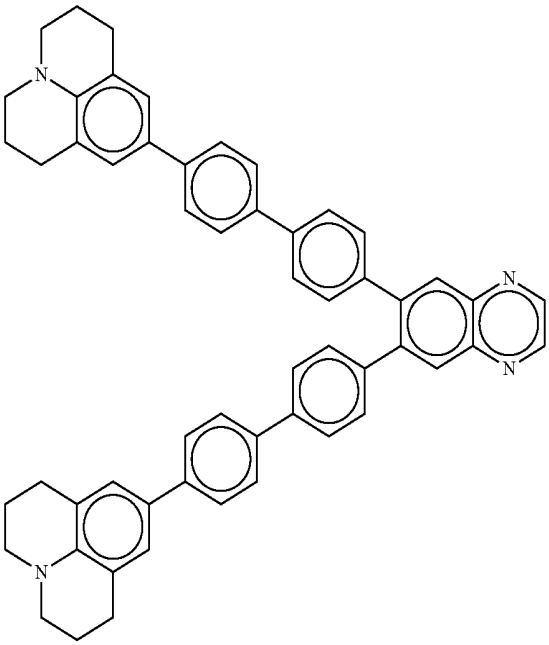
N15



N16

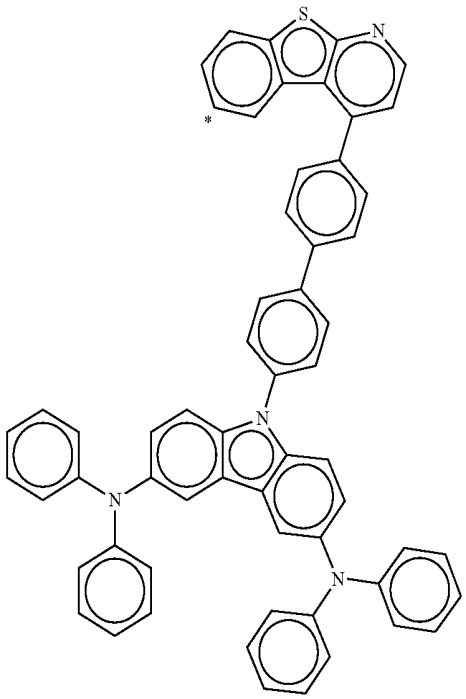
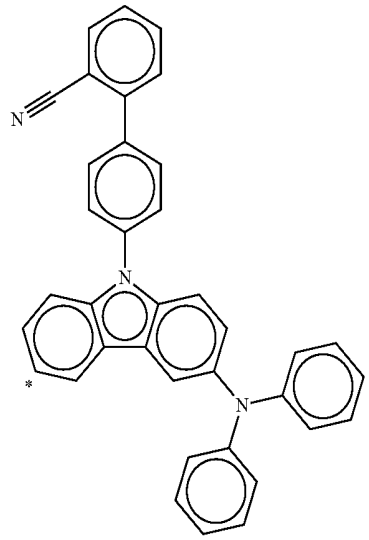


TABLE N-continued

N17



N18

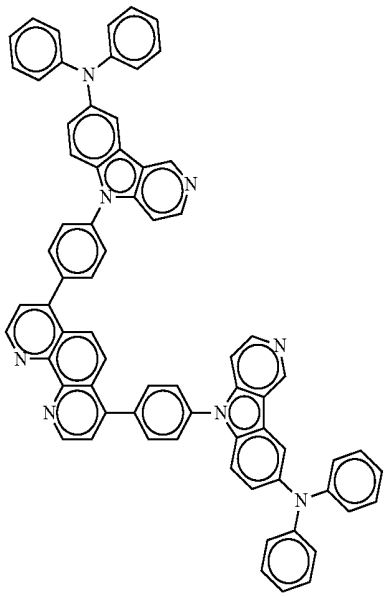
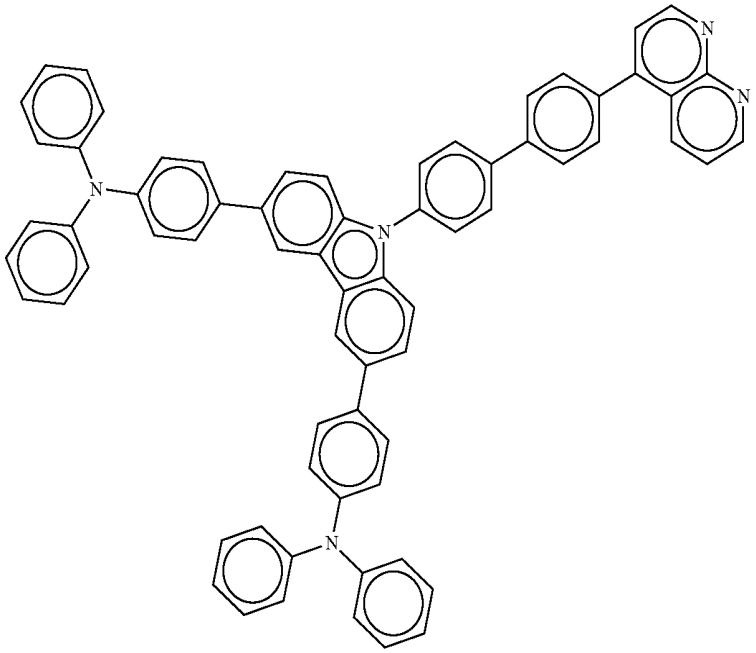
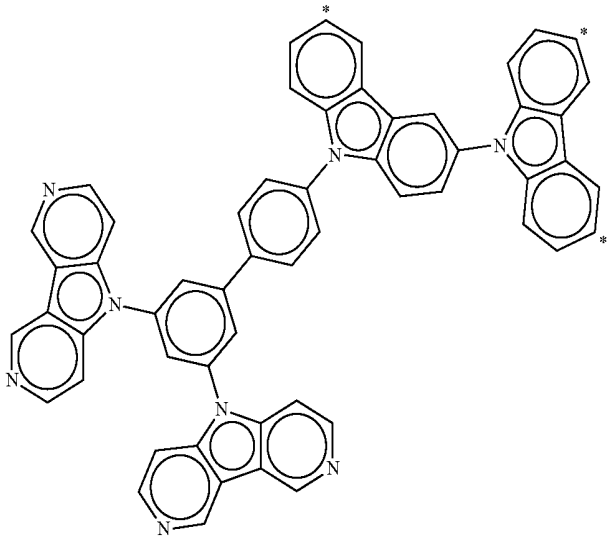


TABLE N-continued

N19



N20



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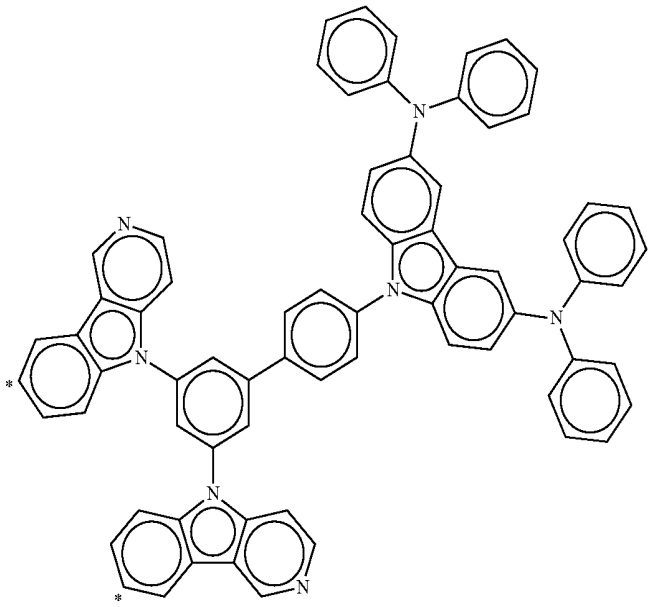
N21



N22

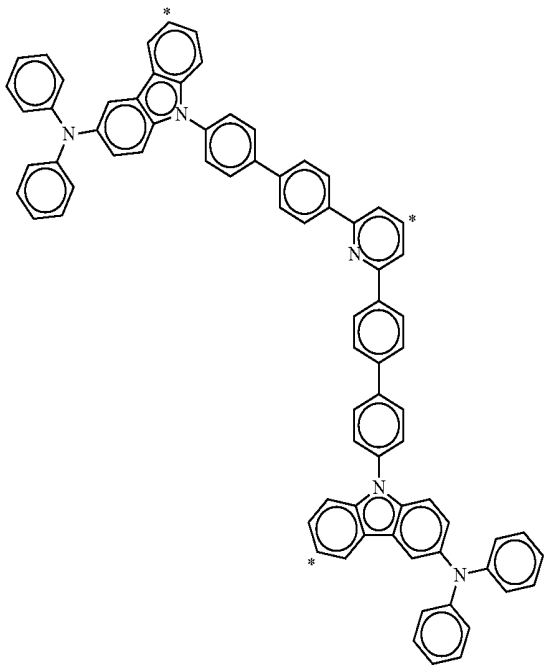
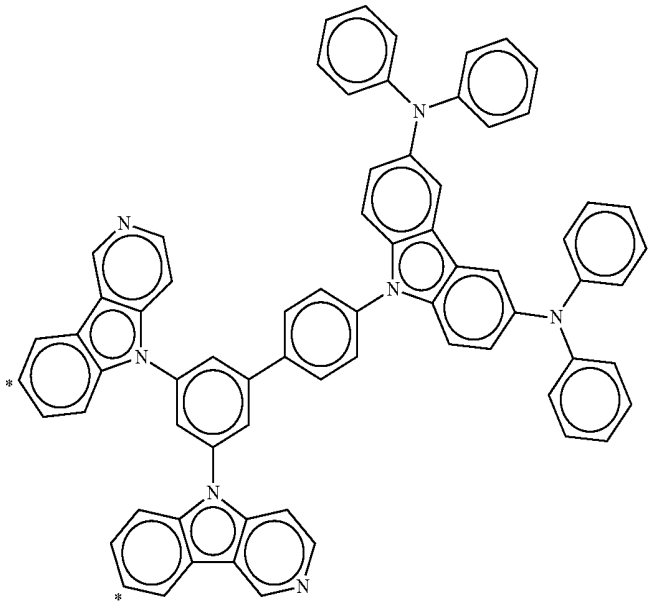


TABLE N-continued

N23



N24

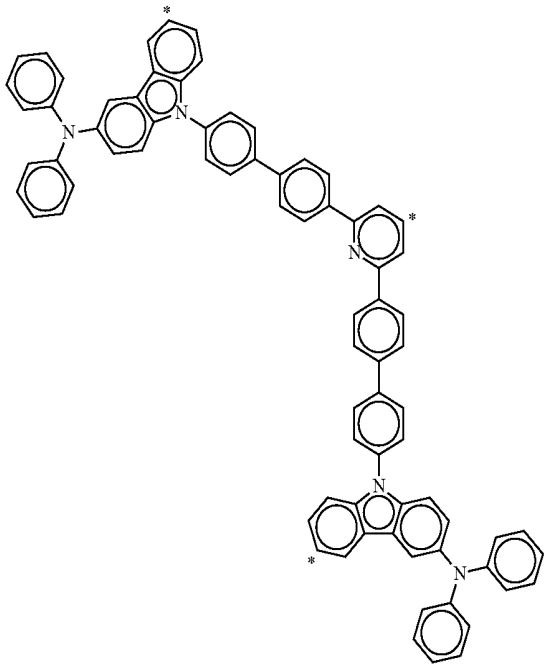
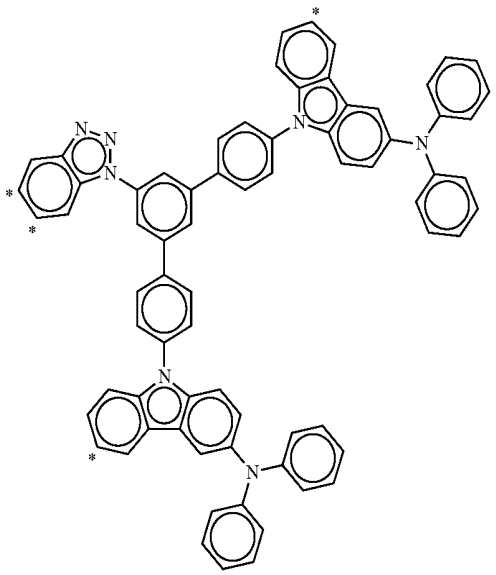
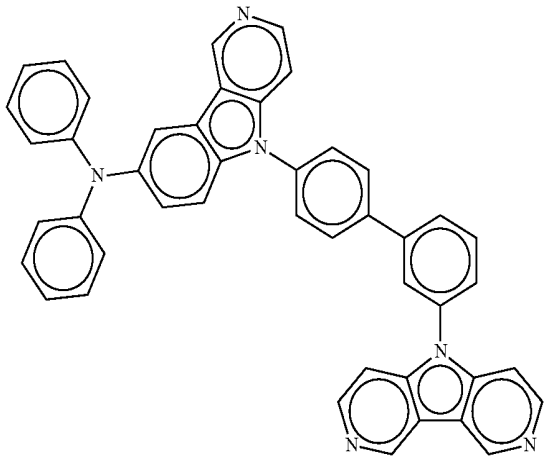


TABLE N-continued

N25



N26



N27

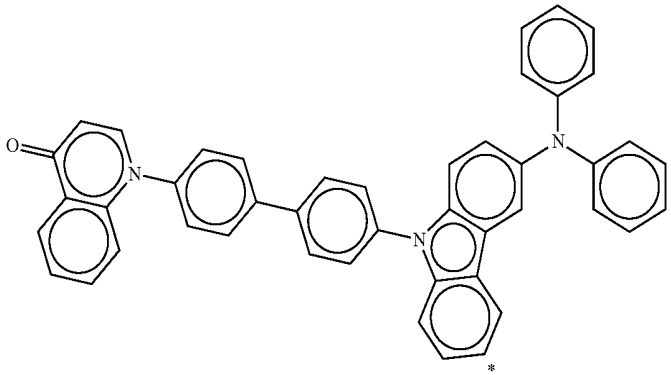
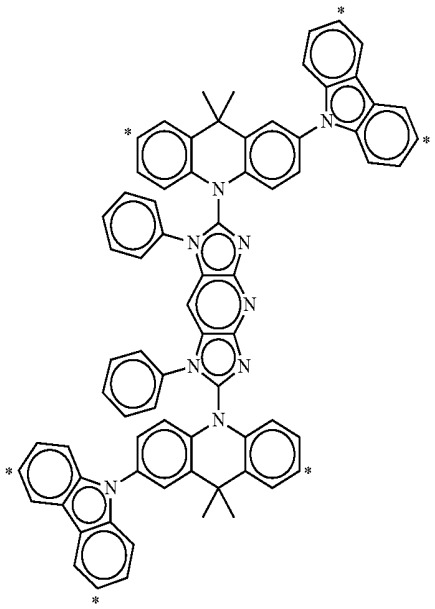


TABLE N-continued

N28



N29

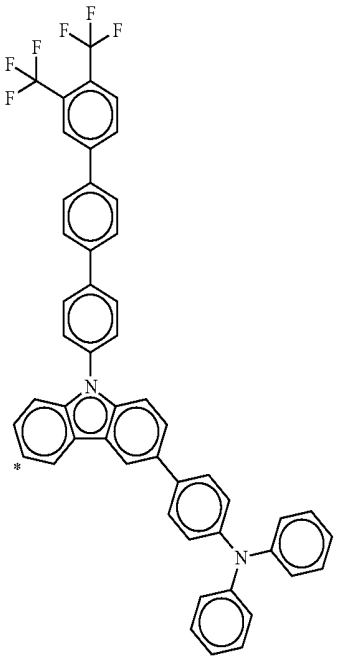
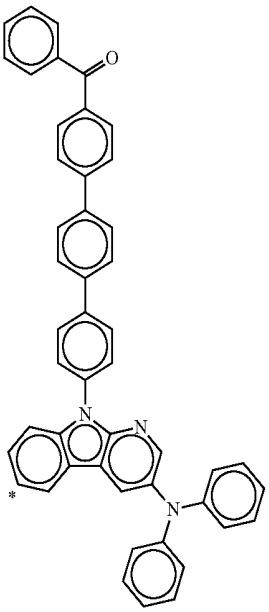
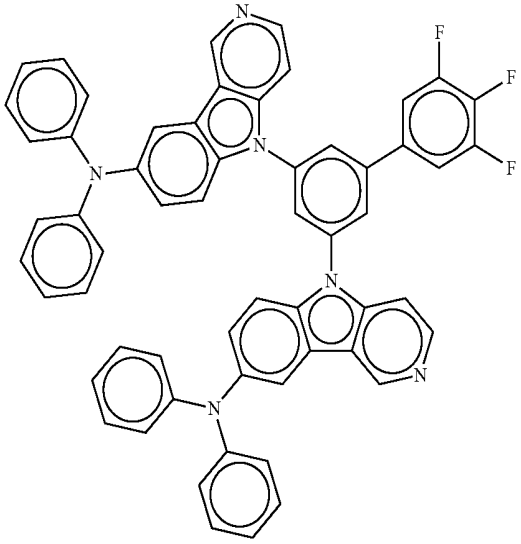


TABLE N-continued

N30



N31



N32

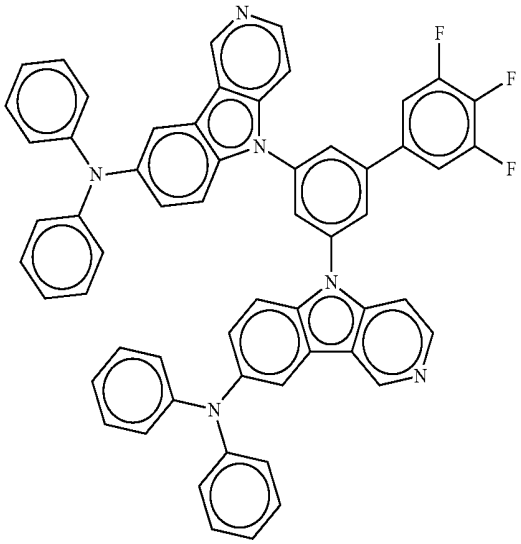
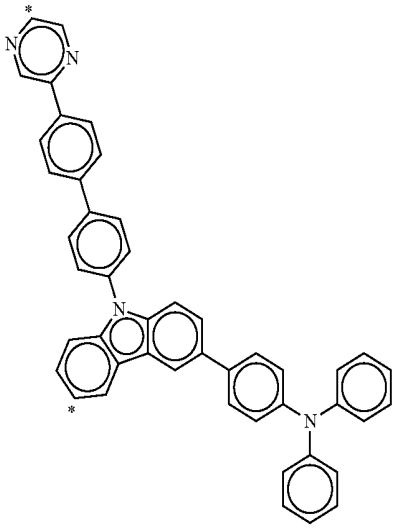


TABLE N-continued

N33



N34

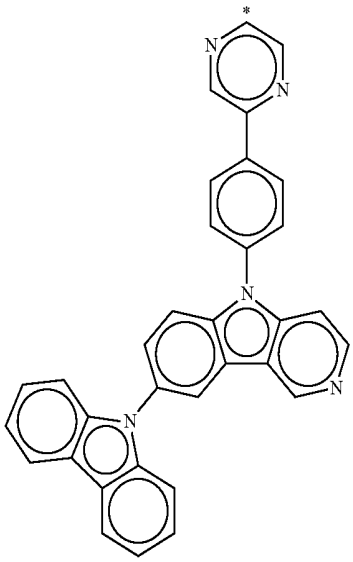
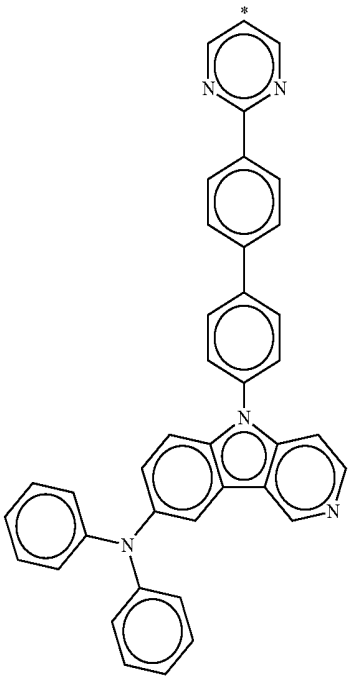


TABLE N-continued

N35



N36

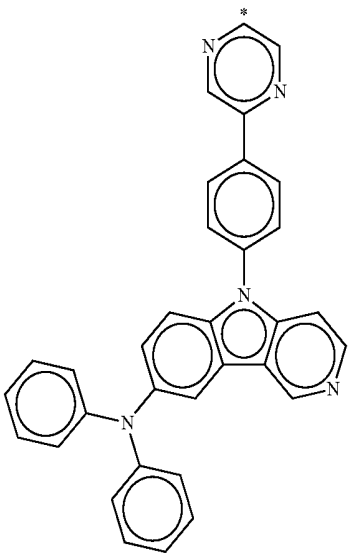
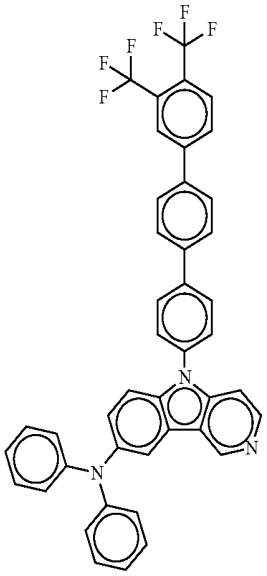


TABLE N-continued

N37



N38

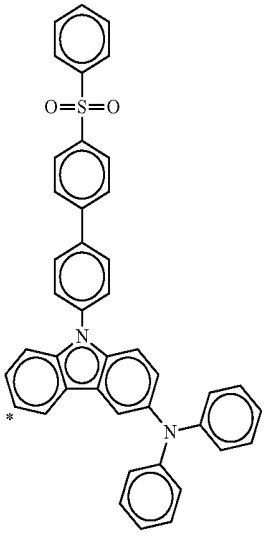
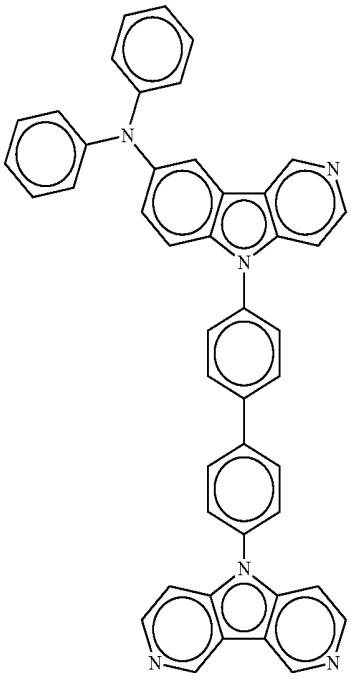


TABLE N-continued

N39



N40

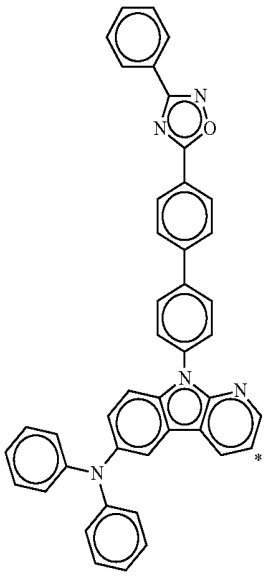
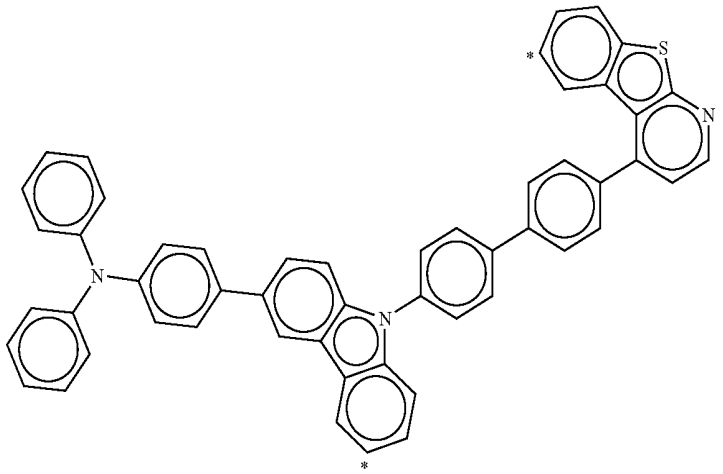
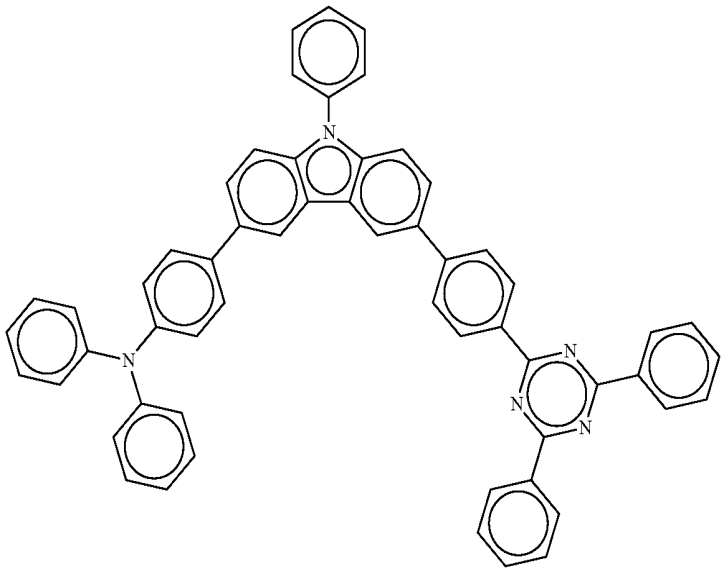


TABLE N-continued

N41



N42



N43

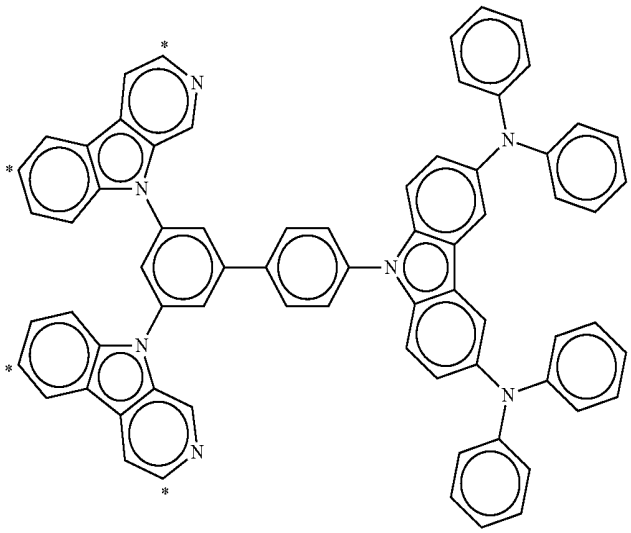
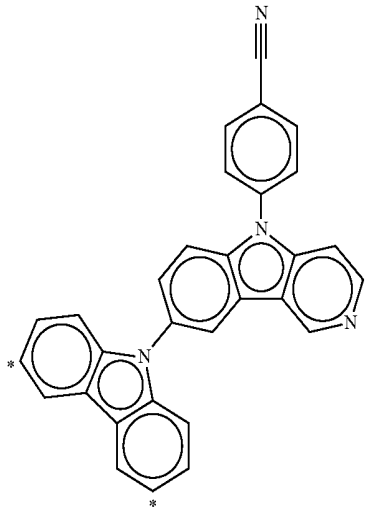
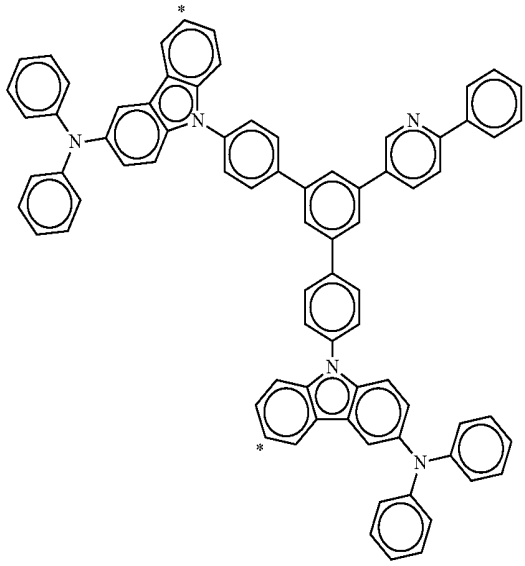


TABLE N-continued

N44



N45



N46

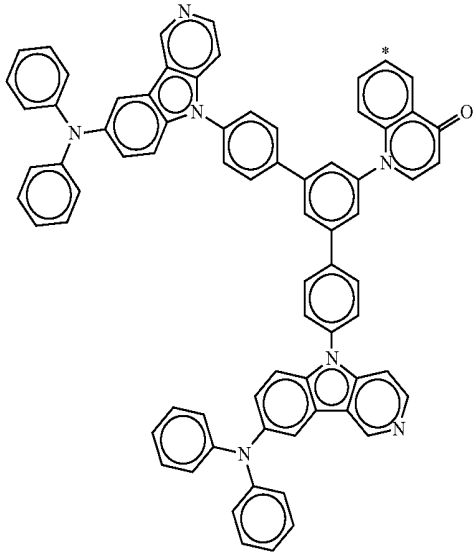
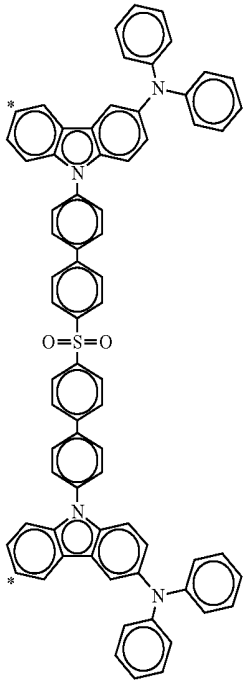


TABLE N-continued

N47



N48

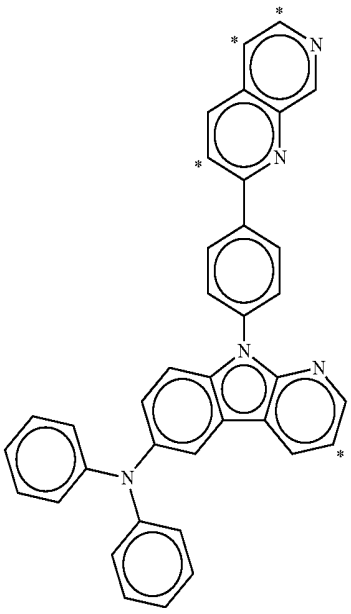
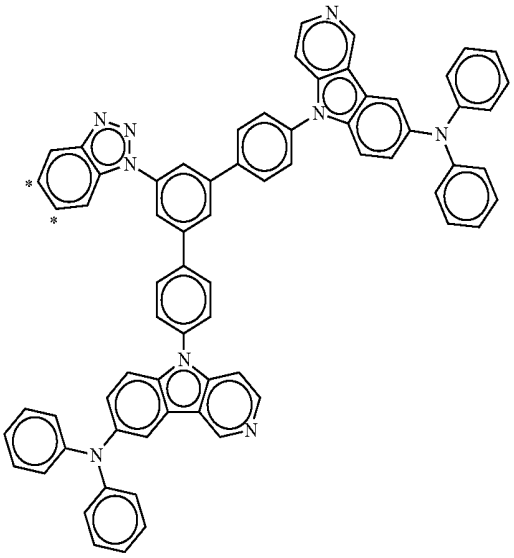


TABLE N-continued

N49



N50

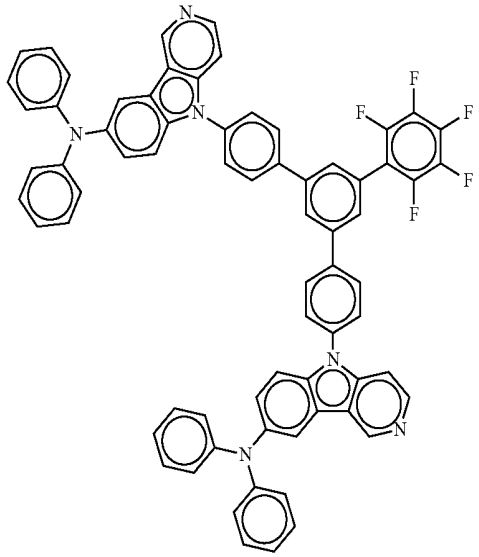
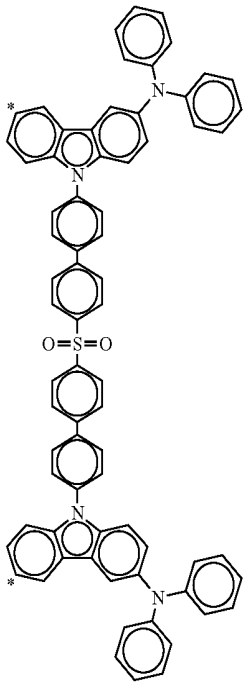
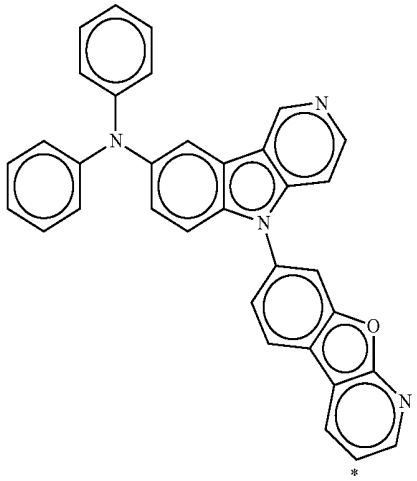


TABLE N-continued

N51



N52



N53

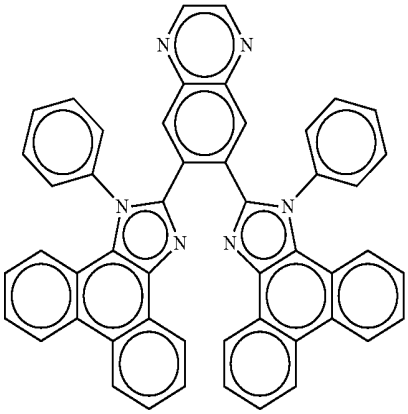
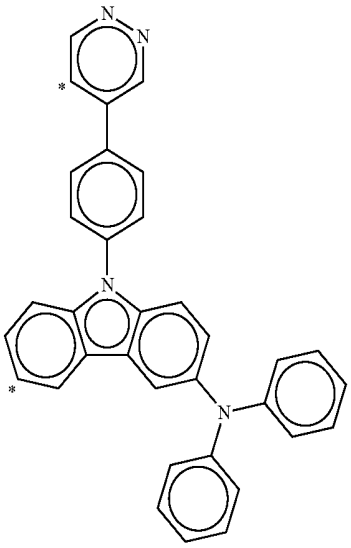


TABLE N-continued

N54



N55

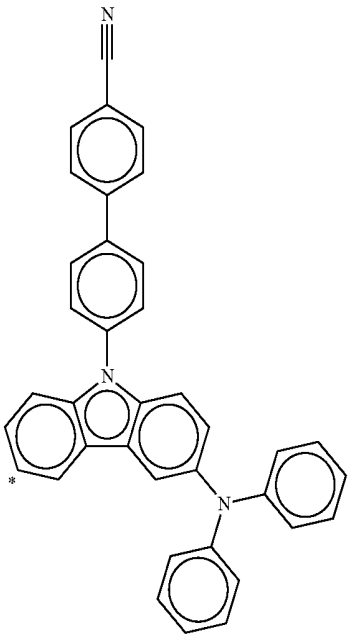
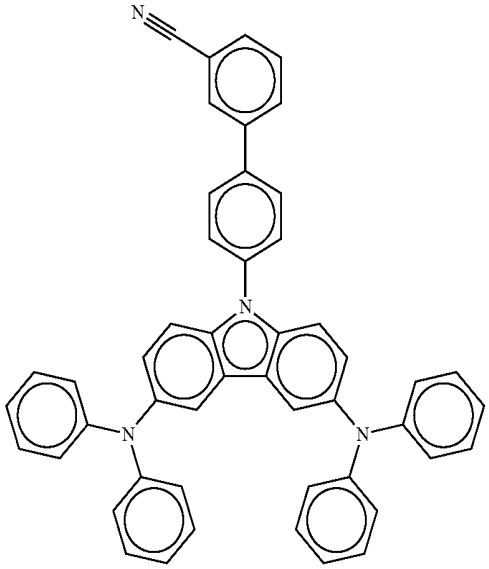


TABLE N-continued

N56



N57

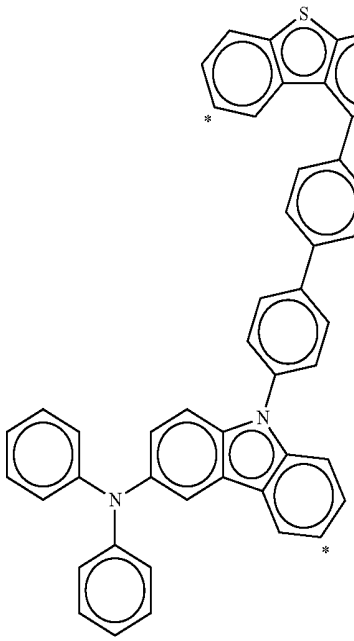
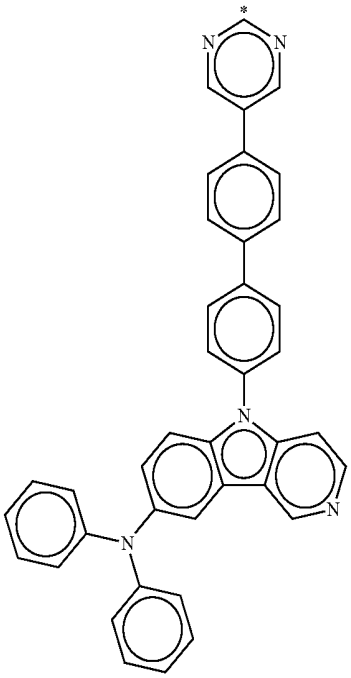


TABLE N-continued

N58



N59

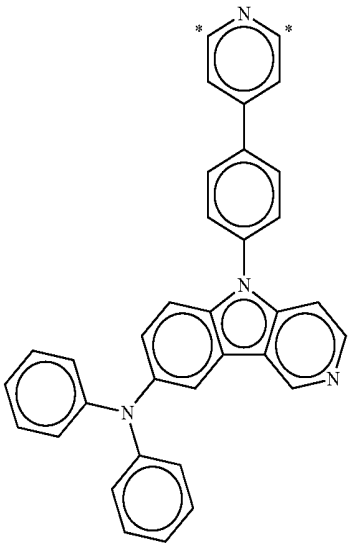
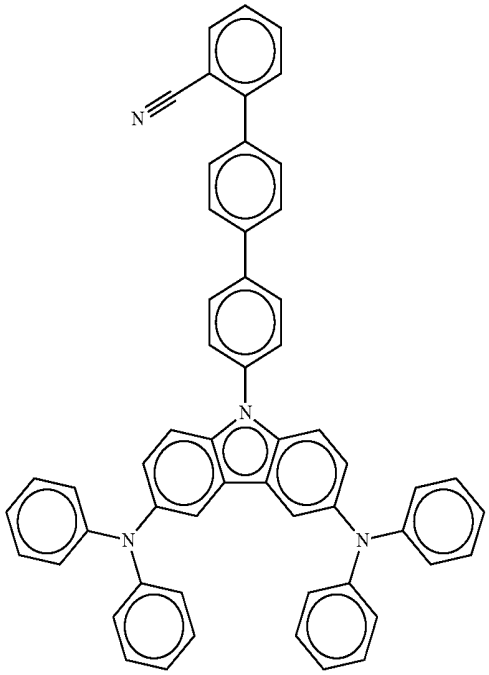


TABLE N-continued

N60



N61

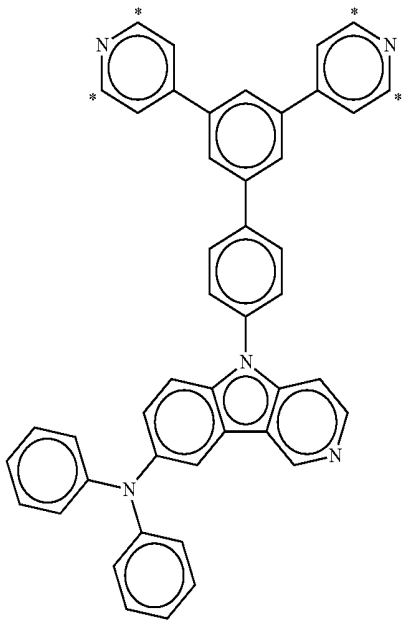
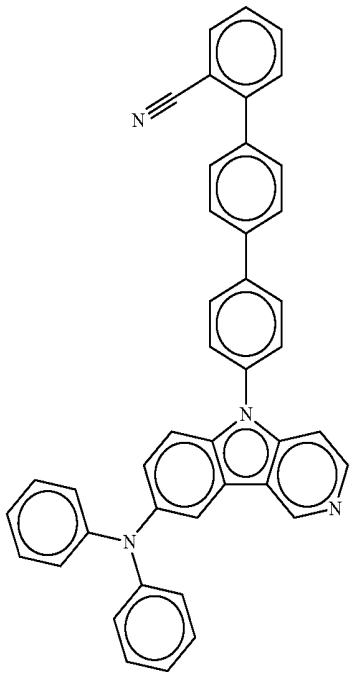
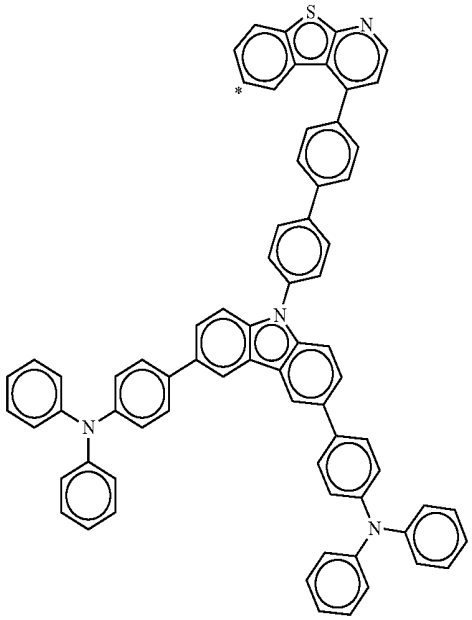


TABLE N-continued

N62



N63



N64

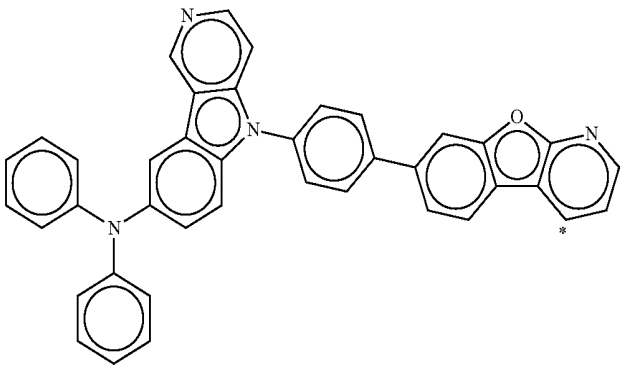
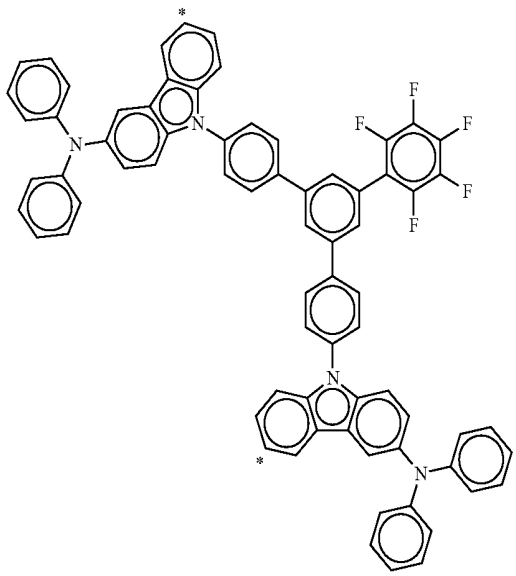


TABLE N-continued

N65



N66

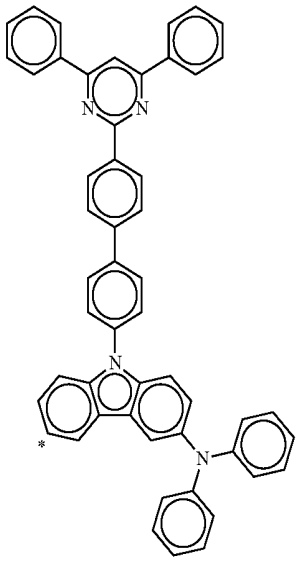
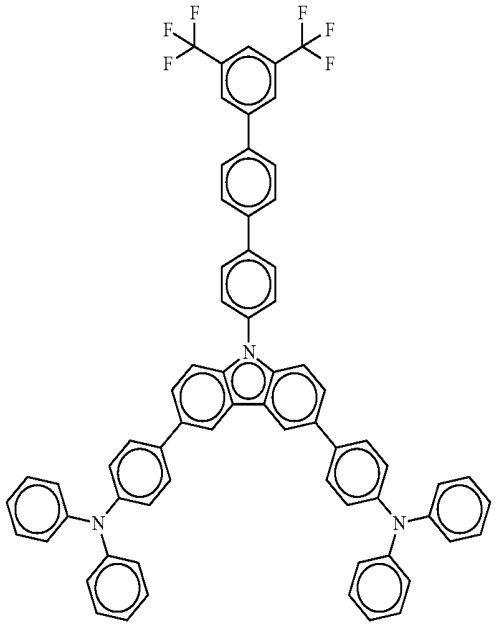
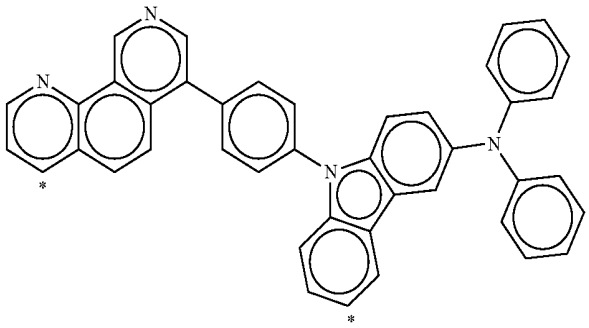


TABLE N-continued

N67



N68



N69

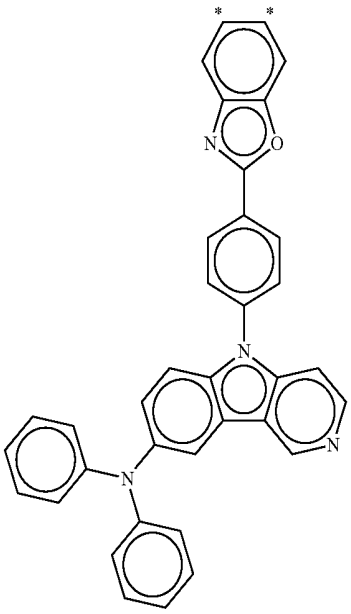
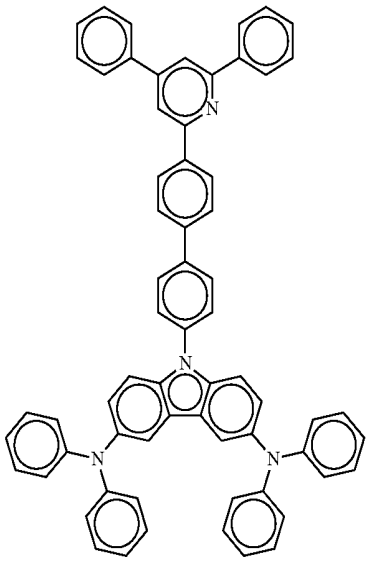


TABLE N-continued

N70



N71

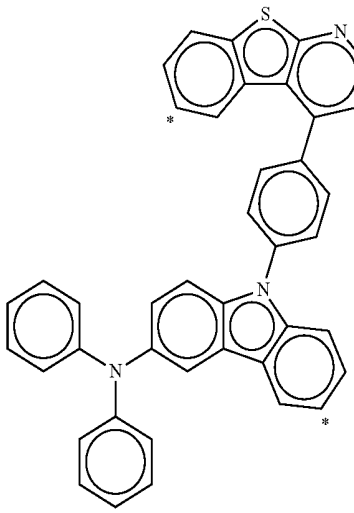
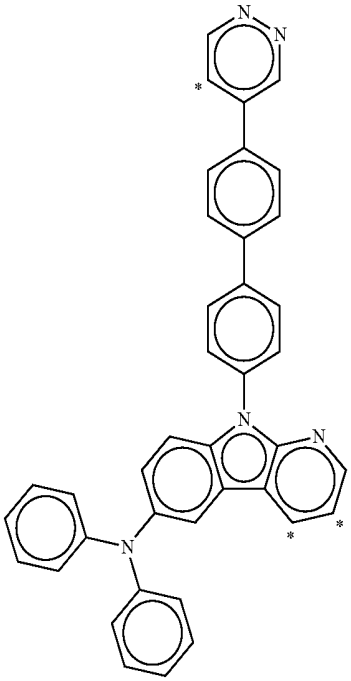


TABLE N-continued

N72



N73

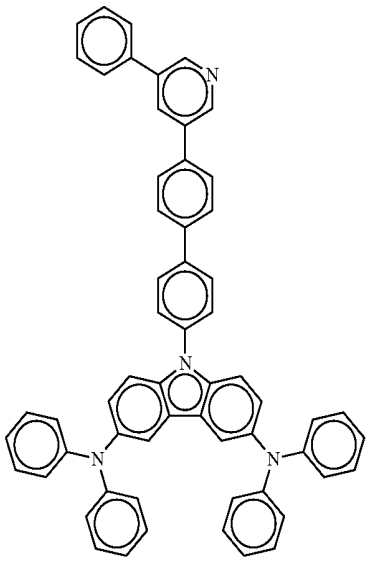
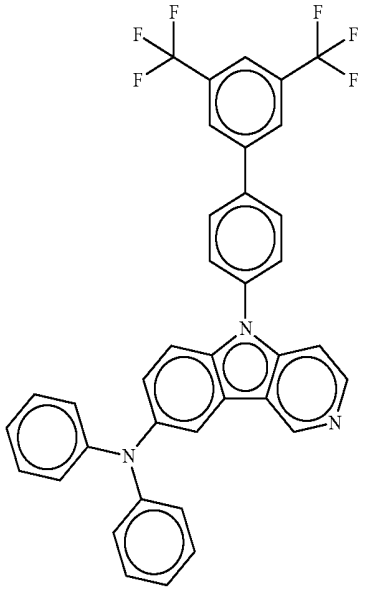


TABLE N-continued

N74



N75

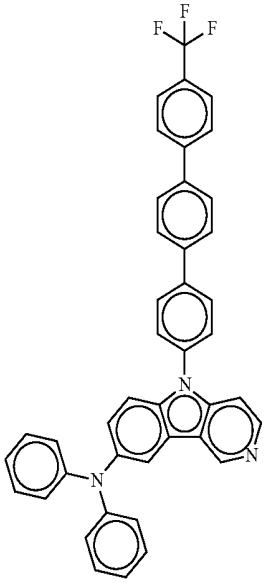
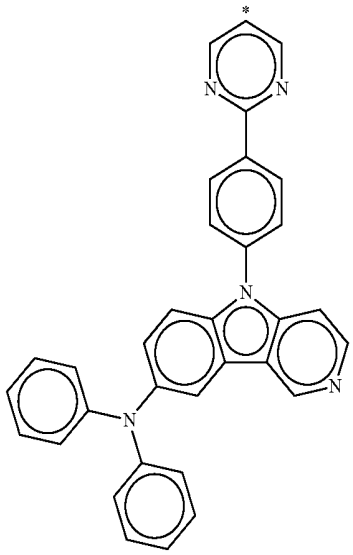
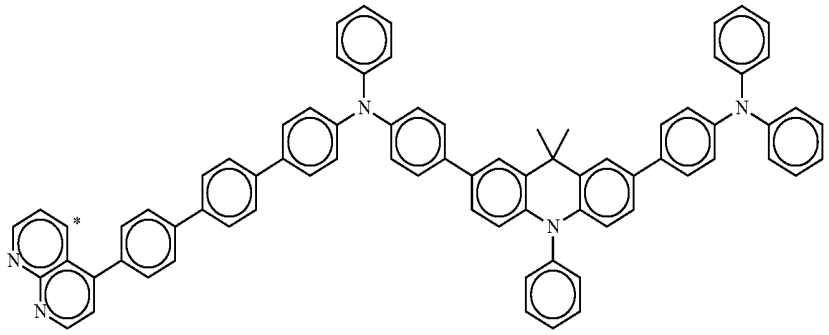


TABLE N-continued

N76



N77



N78

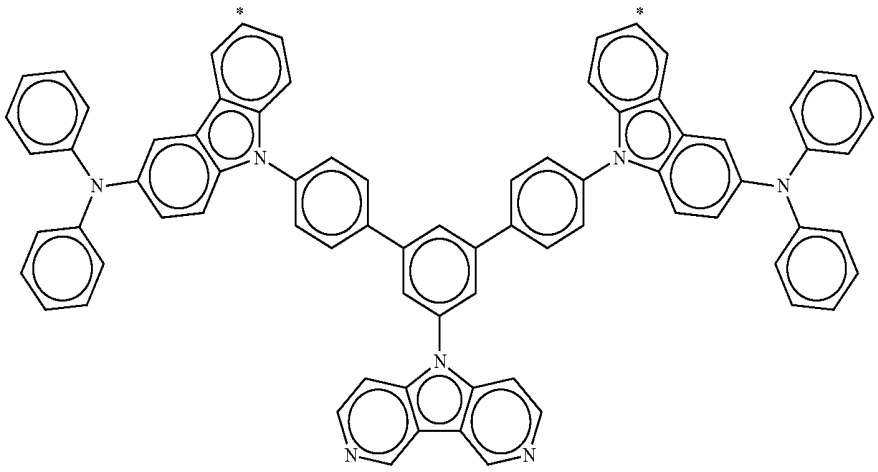
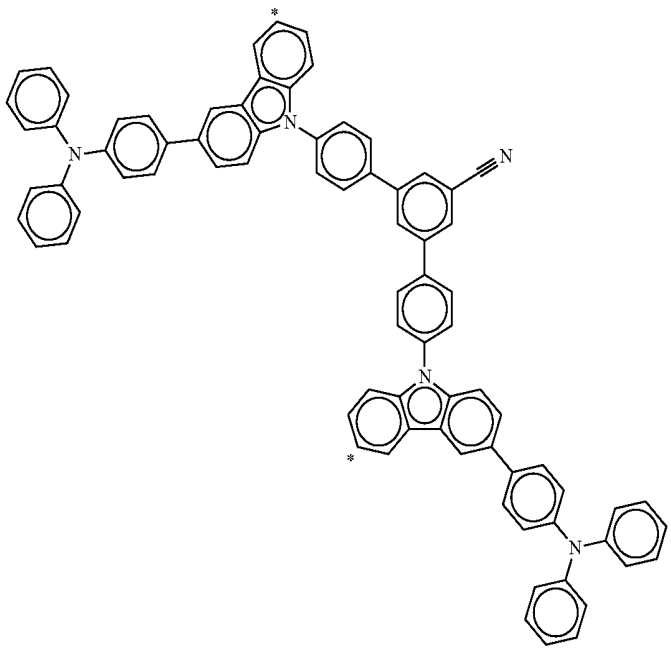


TABLE N-continued

N79



N80

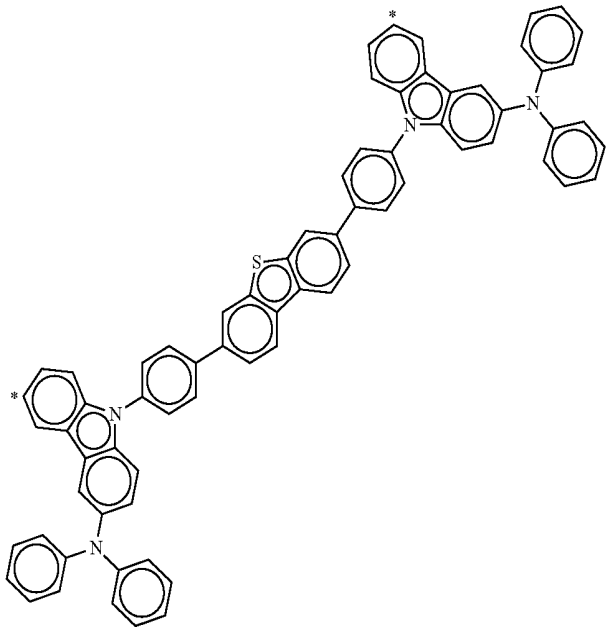
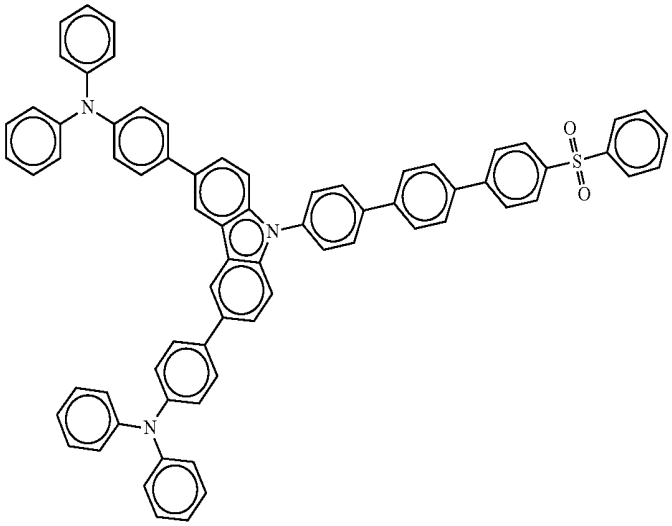
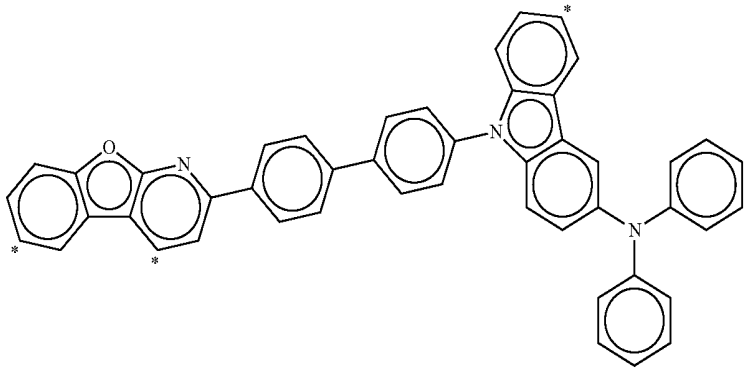


TABLE N-continued

N81



N82



N83

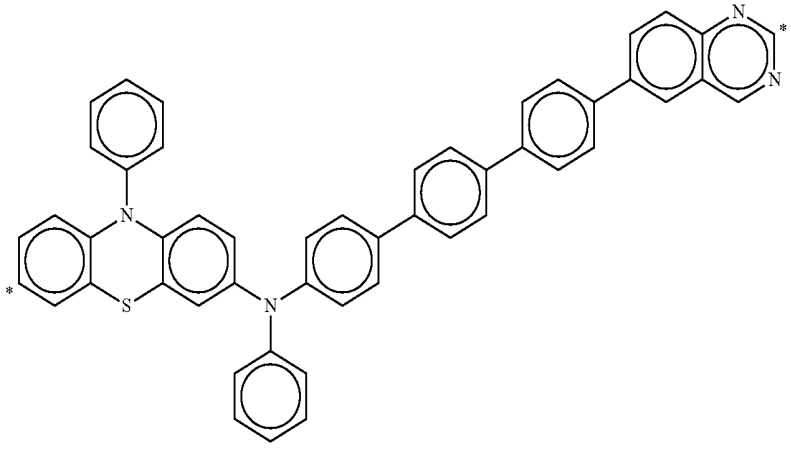
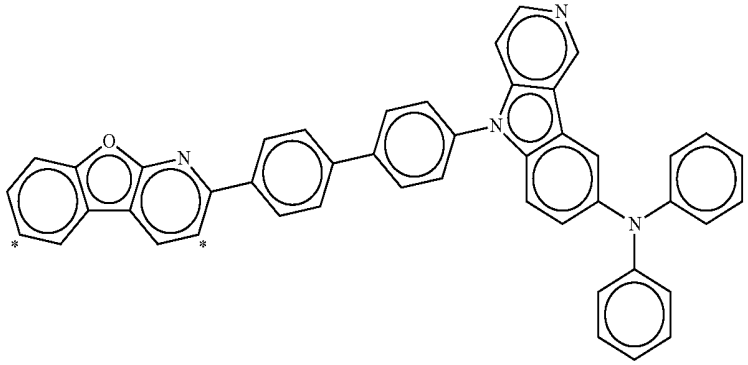
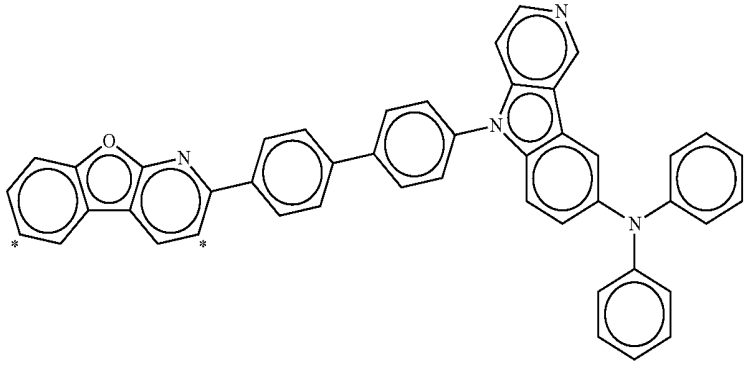


TABLE N-continued

N84



N85



N86

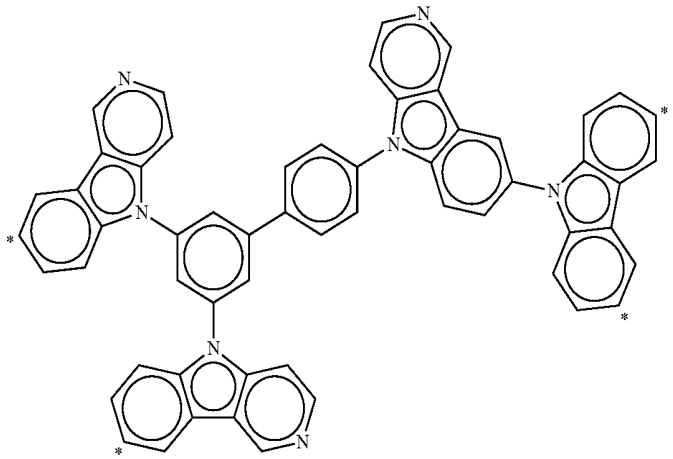
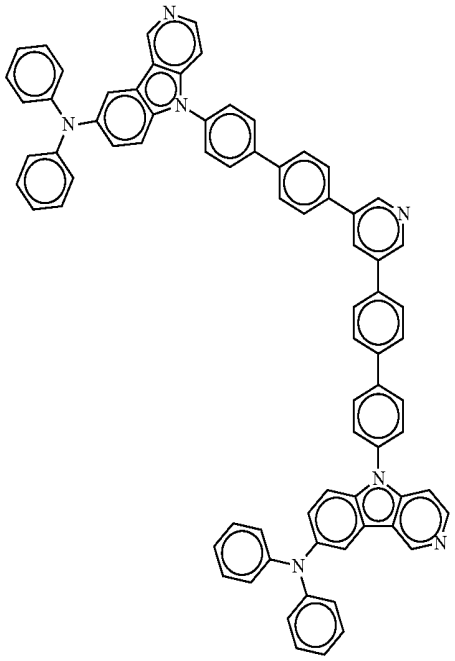


TABLE N-continued

N87



N88

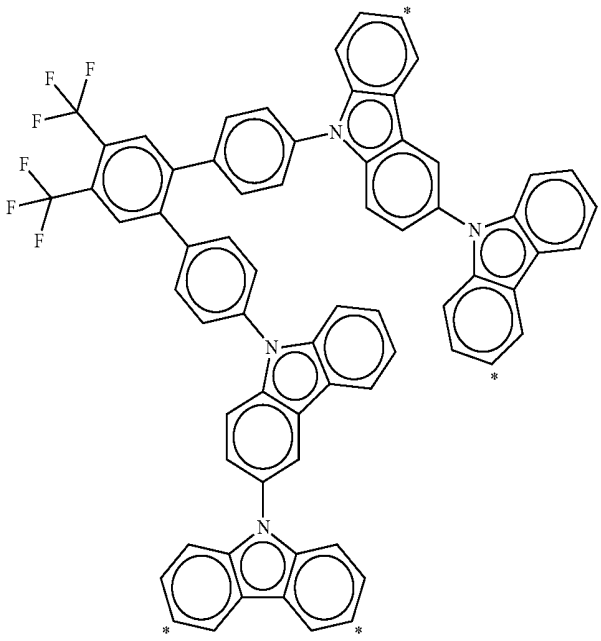
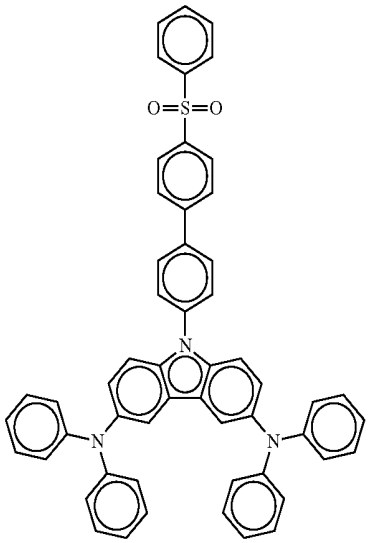
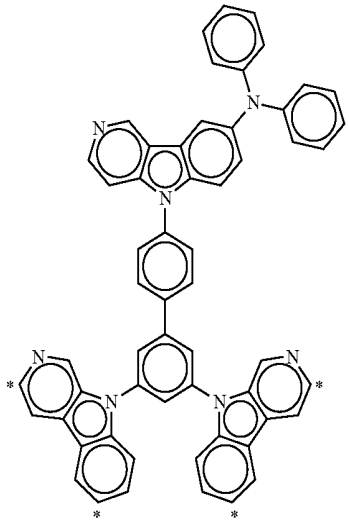


TABLE N-continued

N89



N90



N91

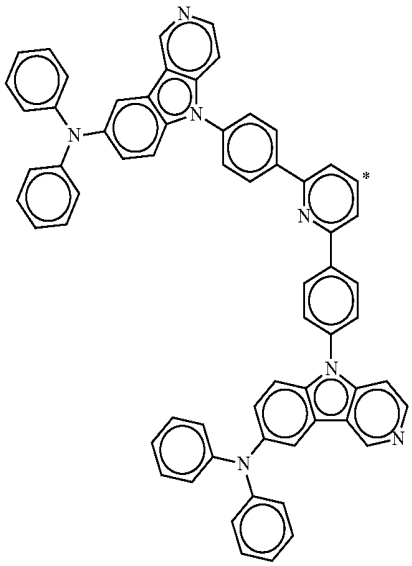
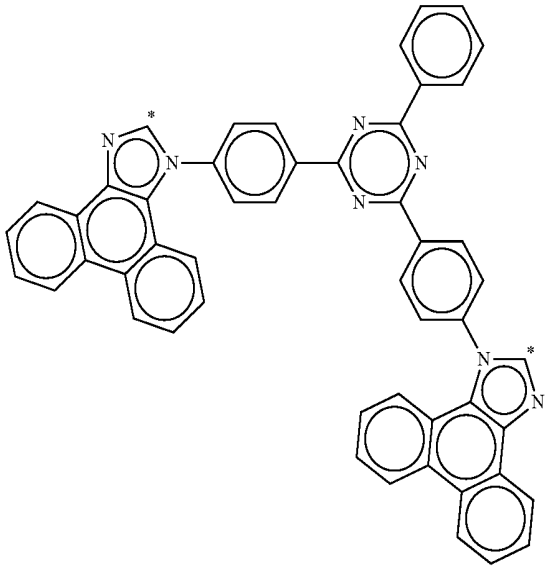


TABLE N-continued

N92



N93

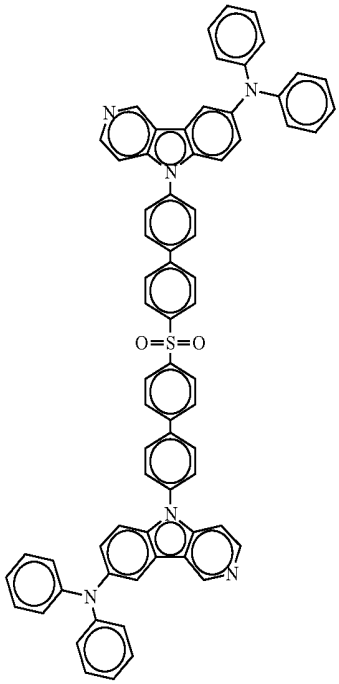
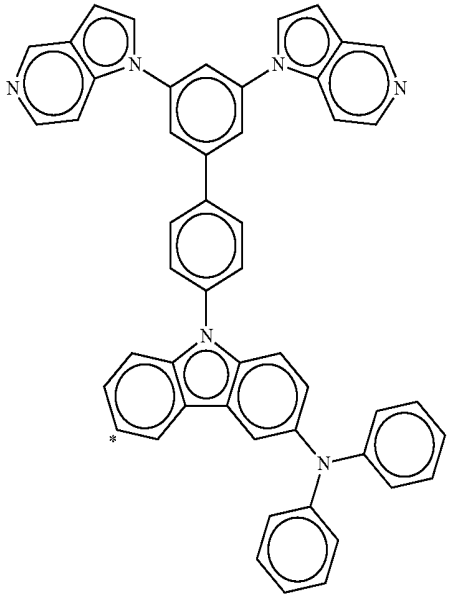


TABLE N-continued

N94



N95

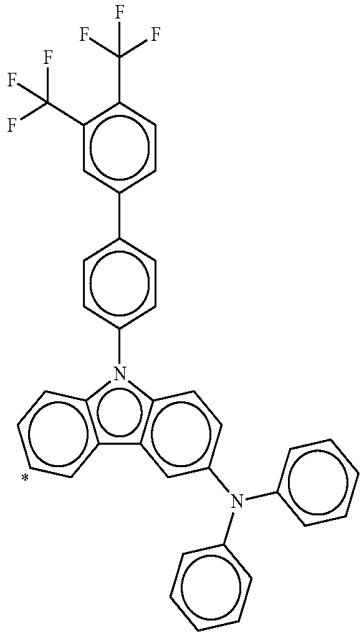


TABLE N-continued

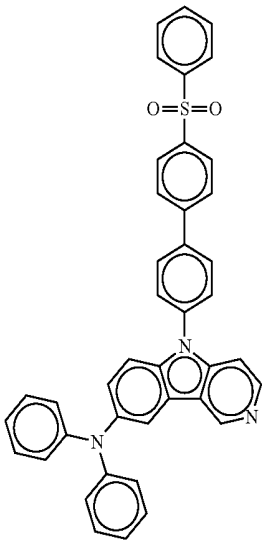
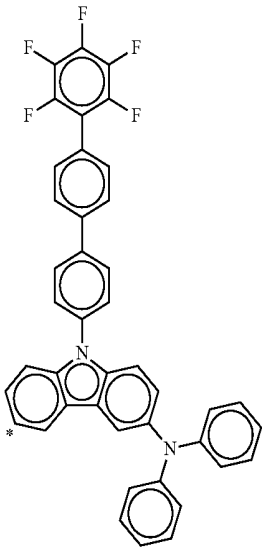
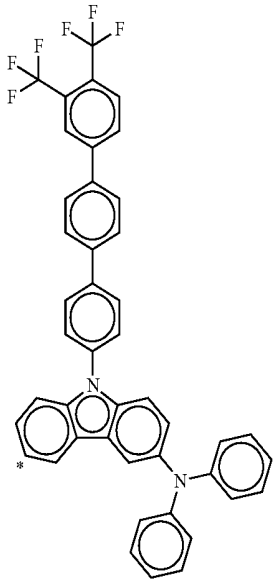
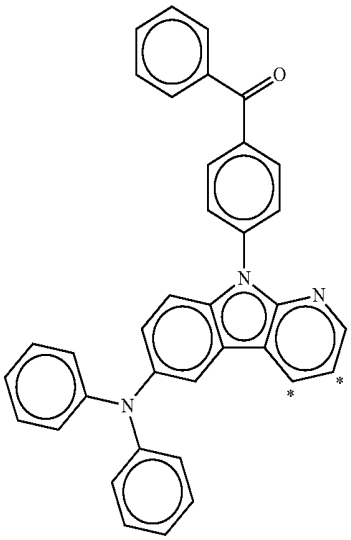
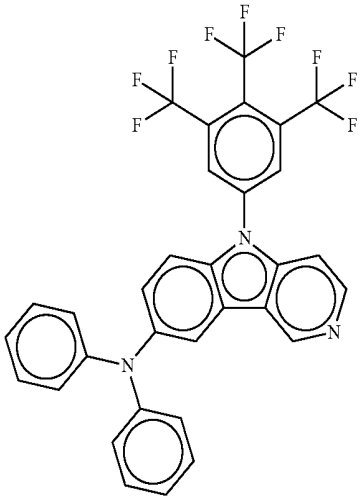
N96	
N97	
N98	

TABLE N-continued

N99



N100



N101

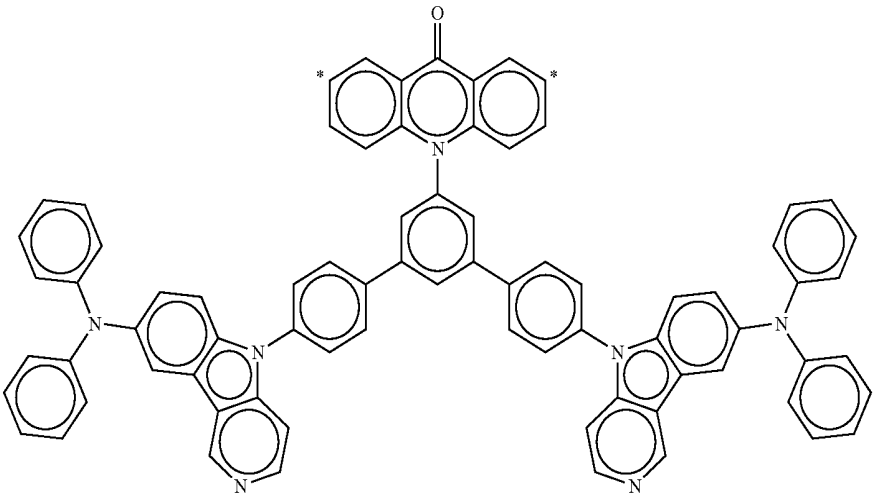
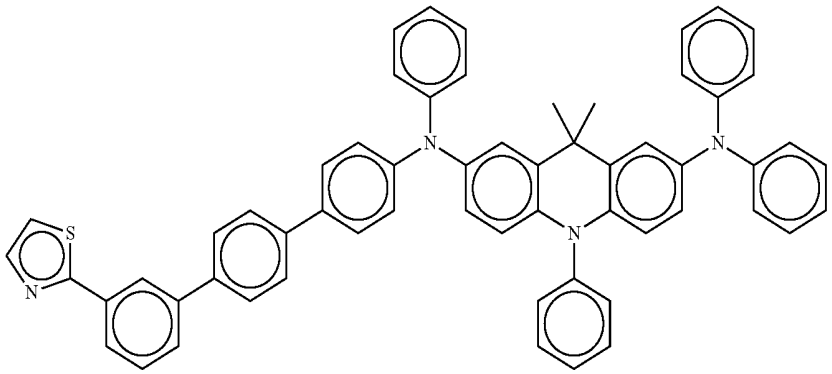
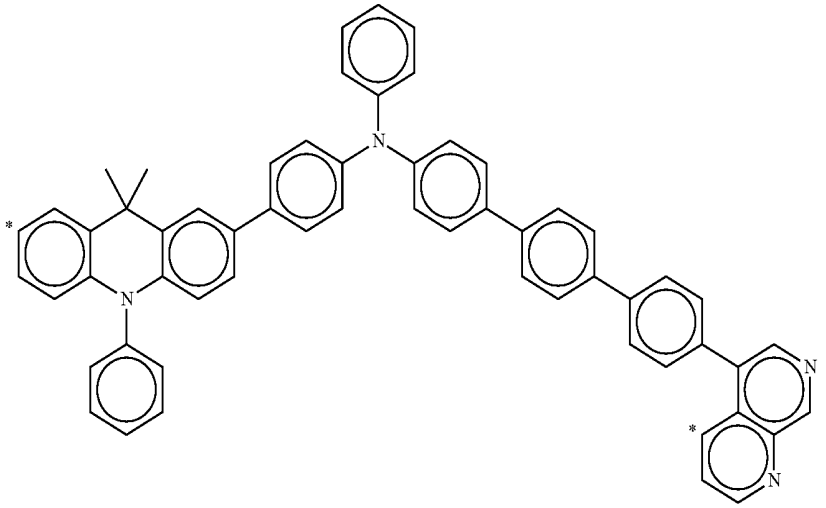


TABLE N-continued

N102



N103



N104

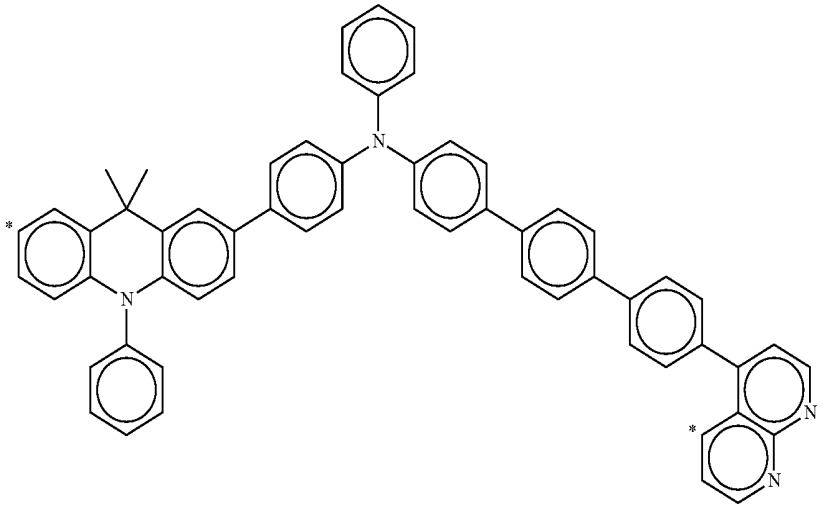
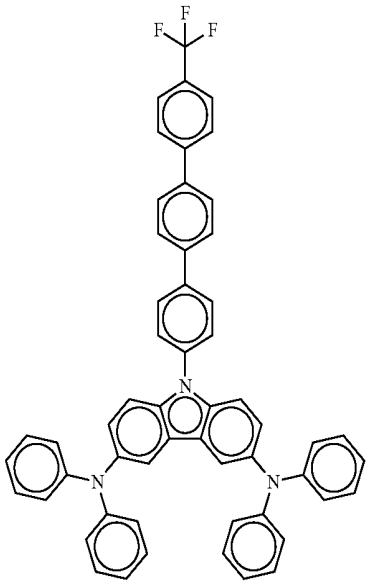
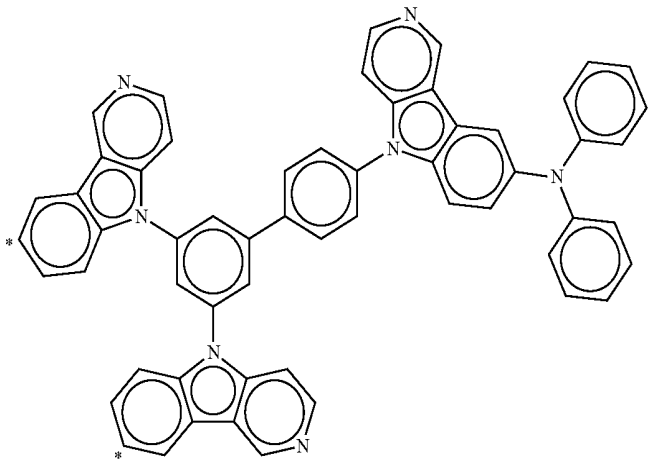


TABLE N-continued

N105



N106



N107

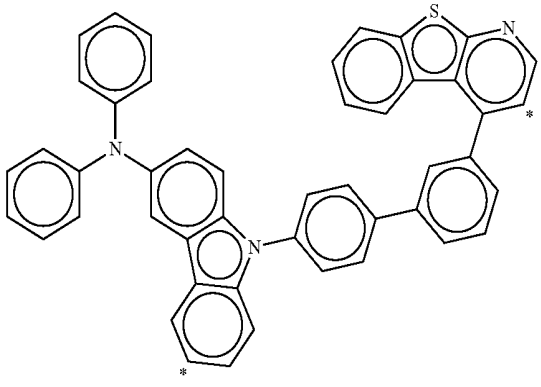
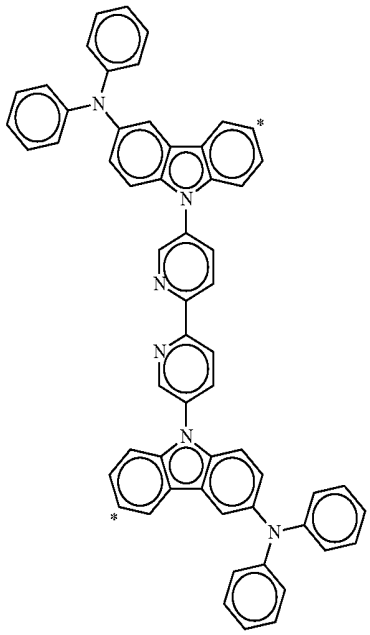


TABLE N-continued

N108



N109

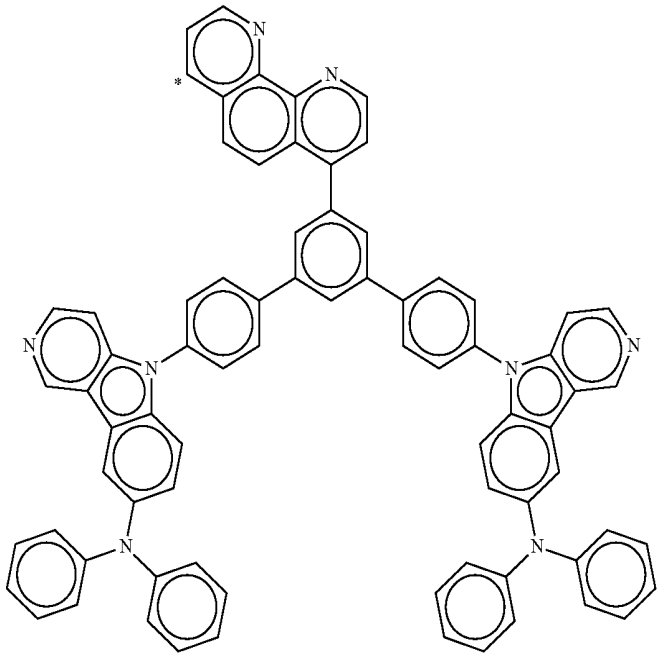
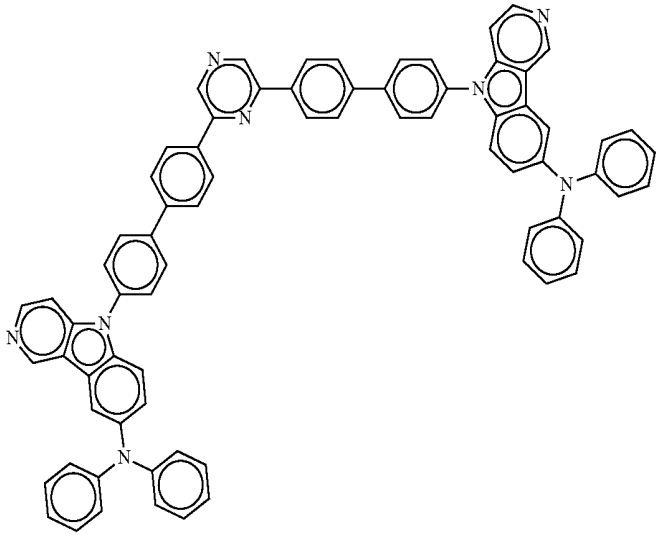
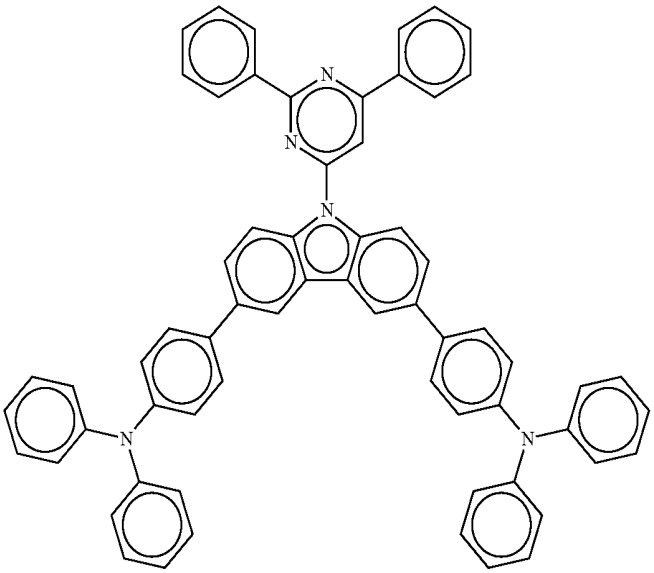


TABLE N-continued

N110



N111



N112

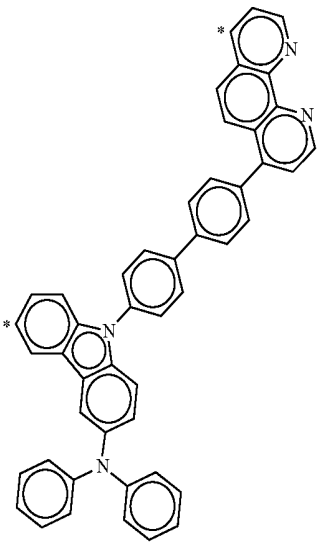
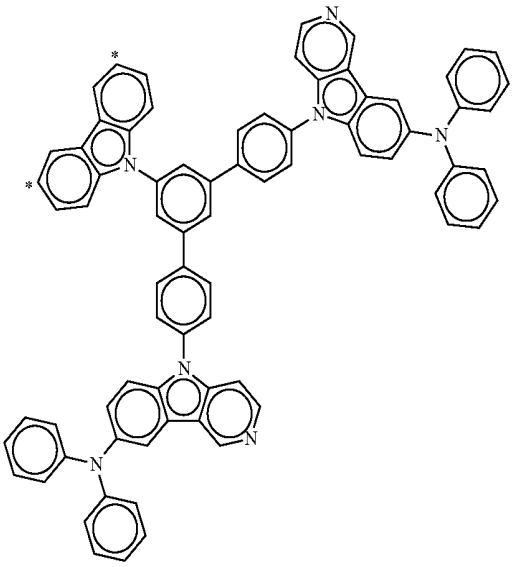


TABLE N-continued

N113



N114

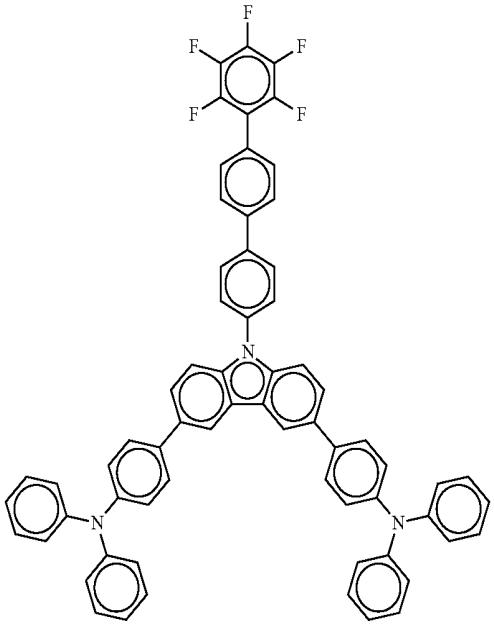
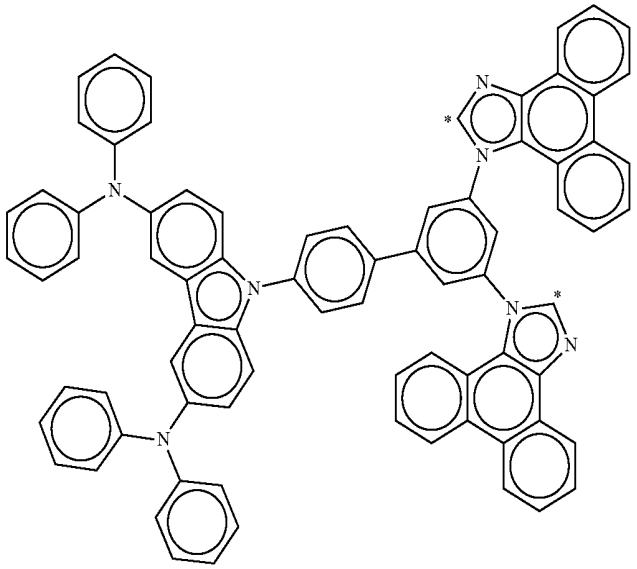


TABLE N-continued

N115



N116

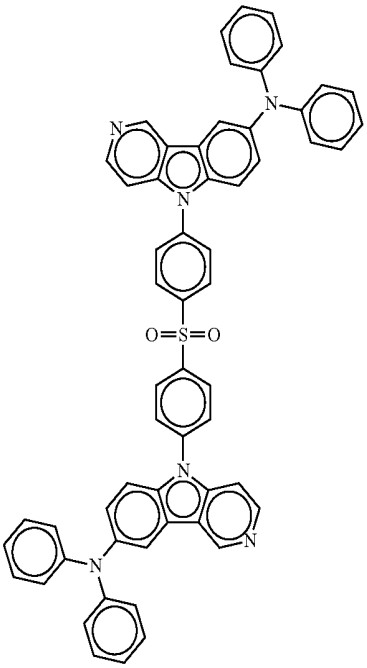
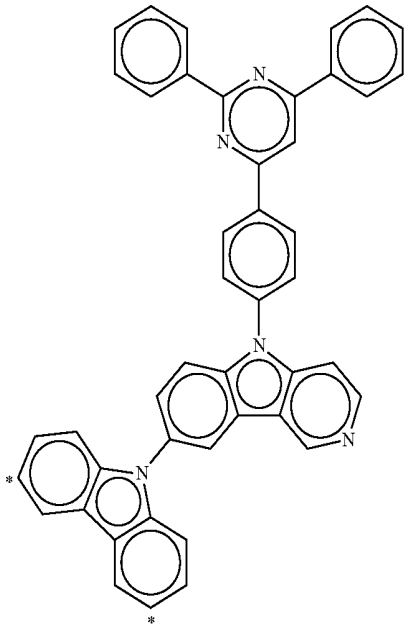


TABLE N-continued

N117



N118

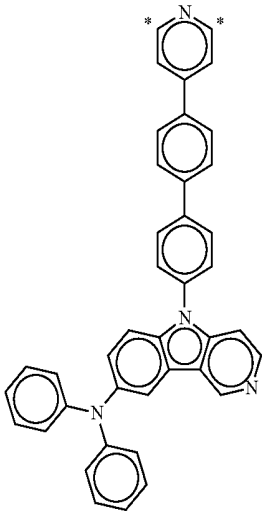
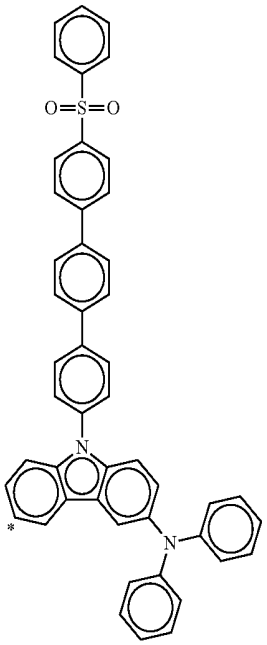


TABLE N-continued

N119



N120

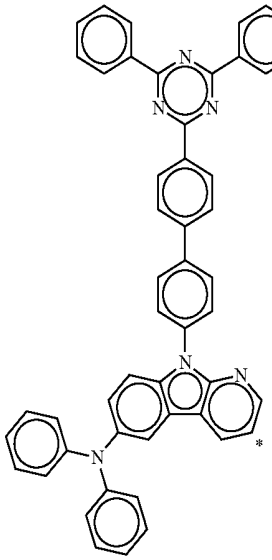
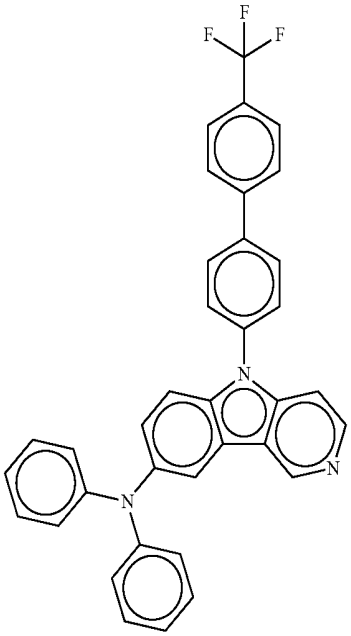


TABLE N-continued

N121



N122

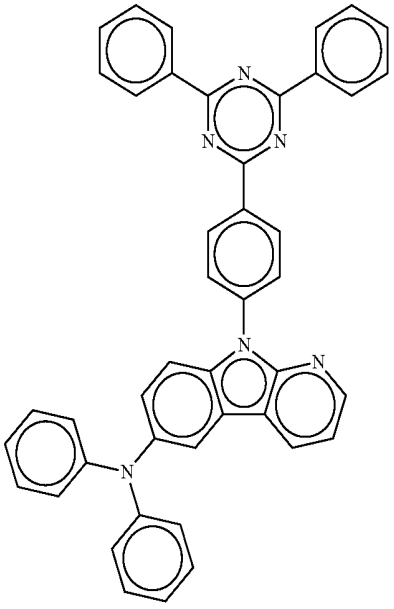
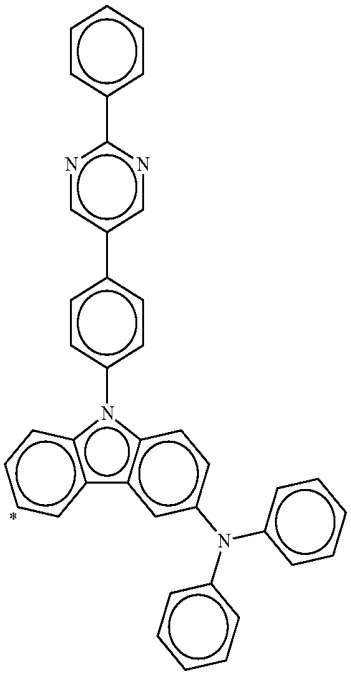


TABLE N-continued

N123



N124

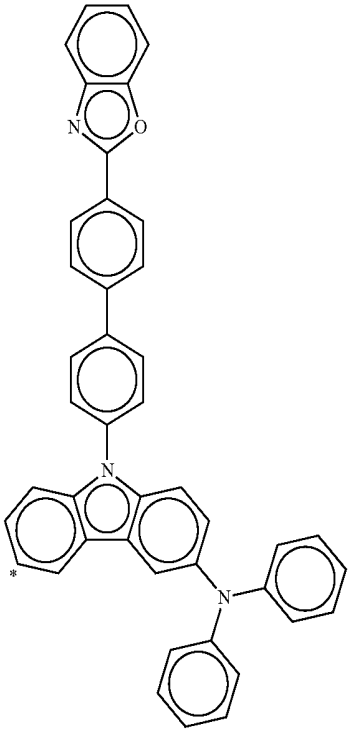
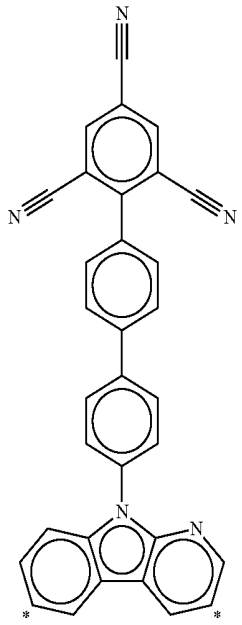


TABLE N-continued

N125



N126

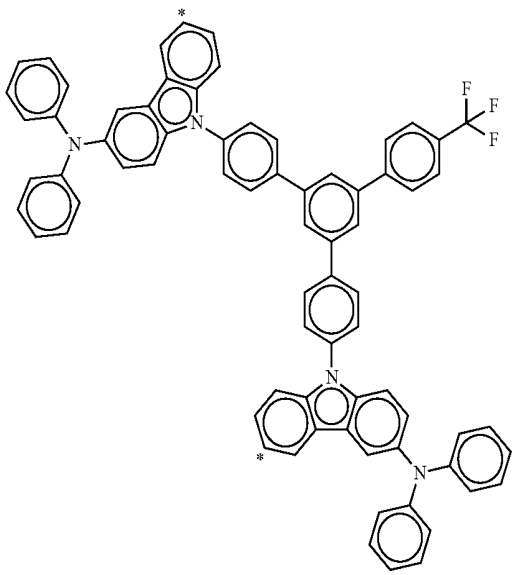
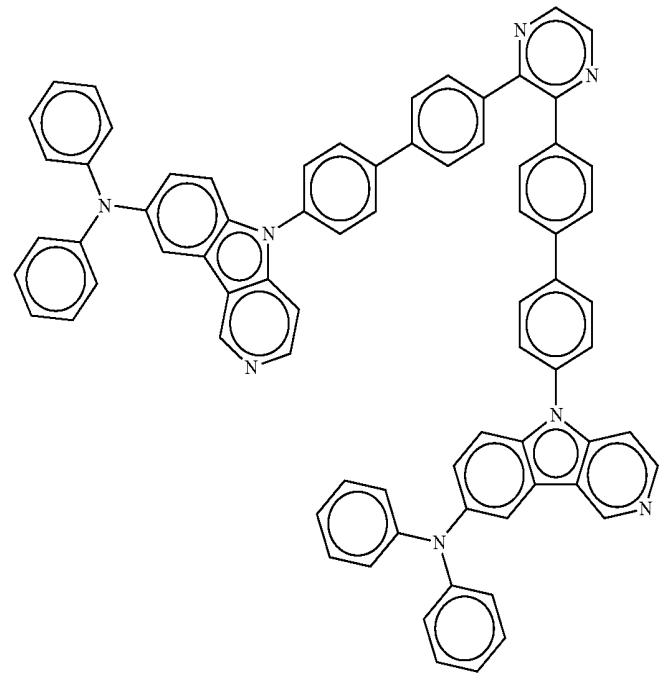
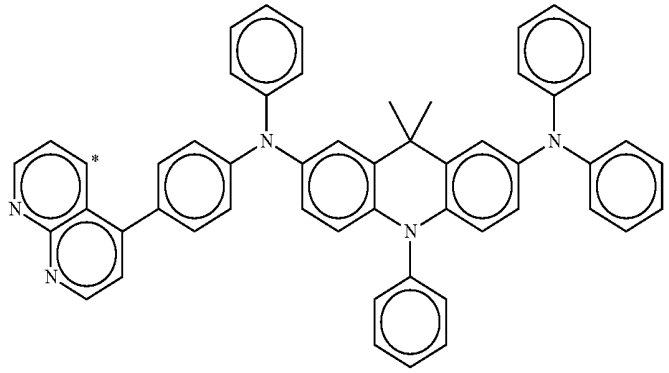


TABLE N-continued

N127



N128



N129

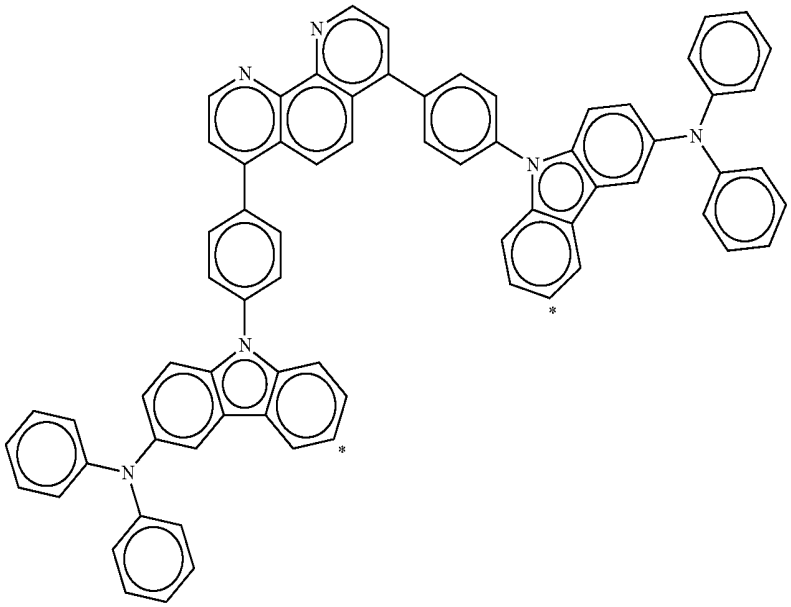
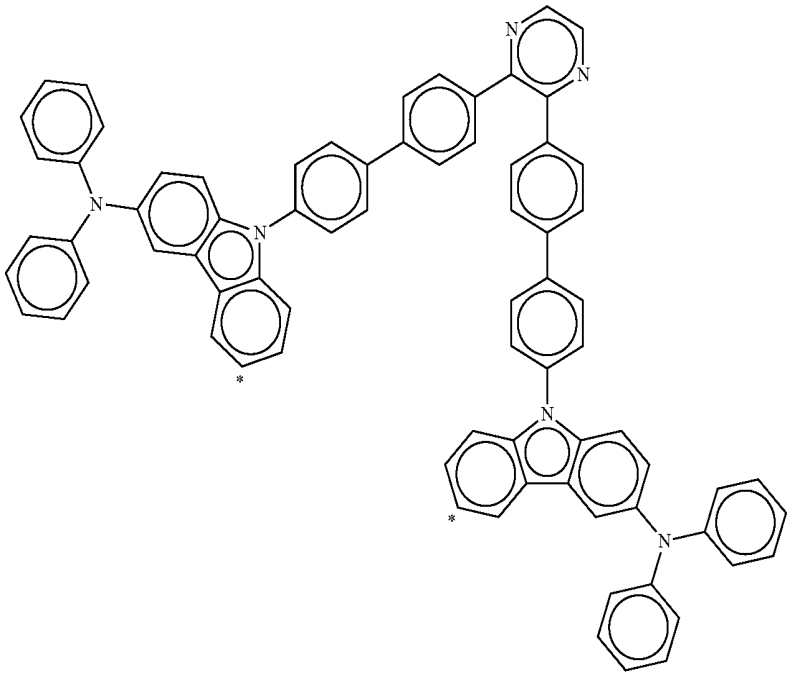


TABLE N-continued

N130



N131

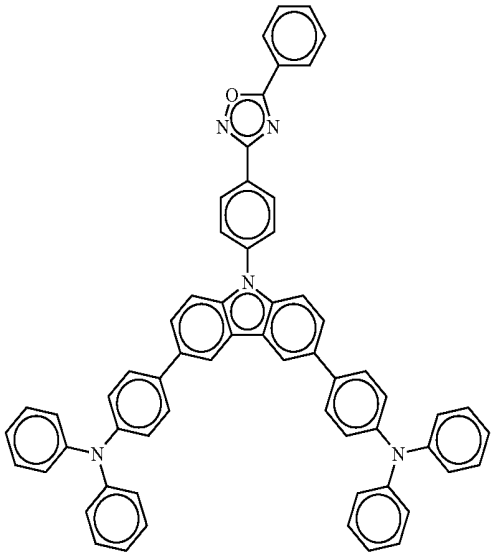
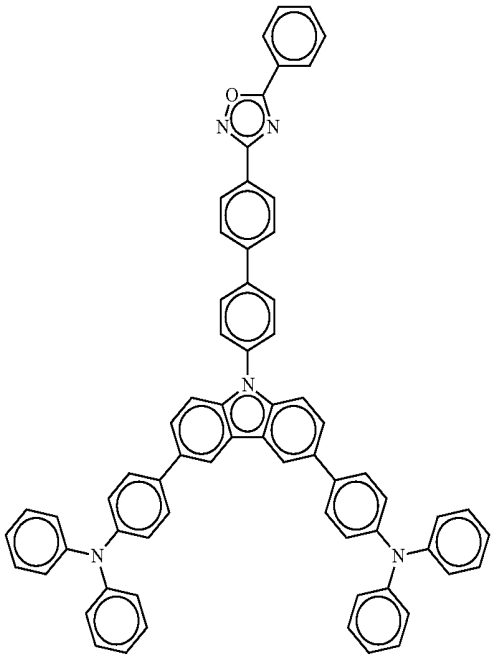
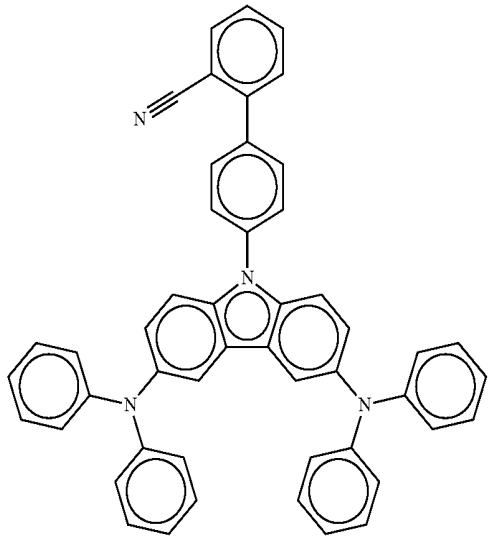


TABLE N-continued

N132



N133



N134

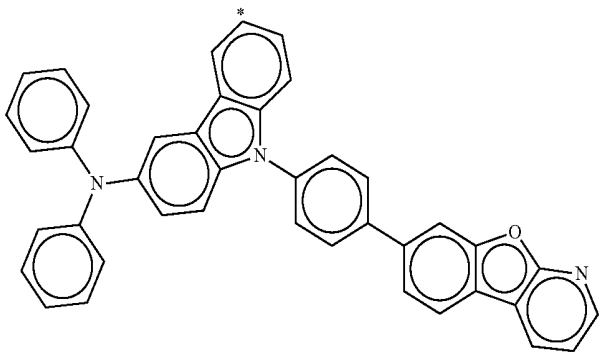
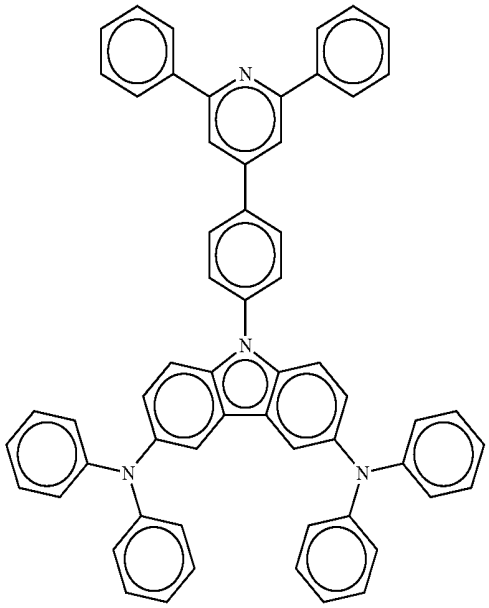
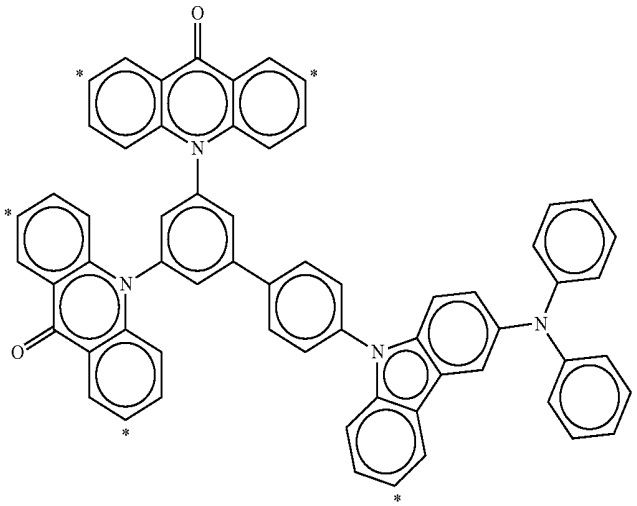


TABLE N-continued

N135



N136



N137

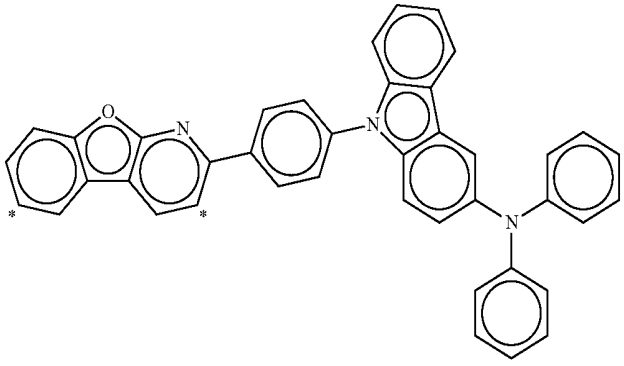
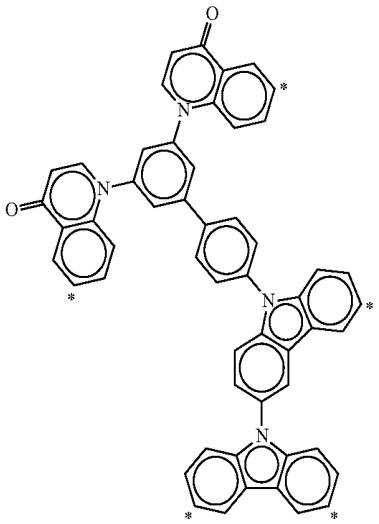


TABLE N-continued

N138



N139

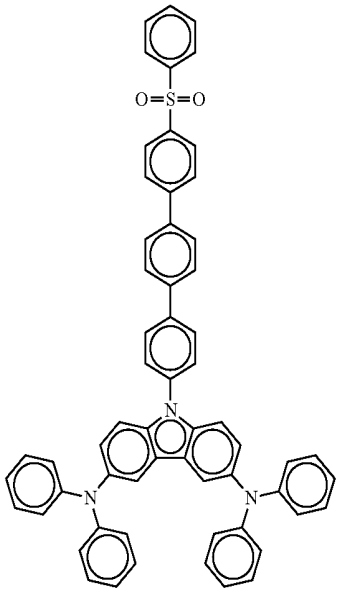
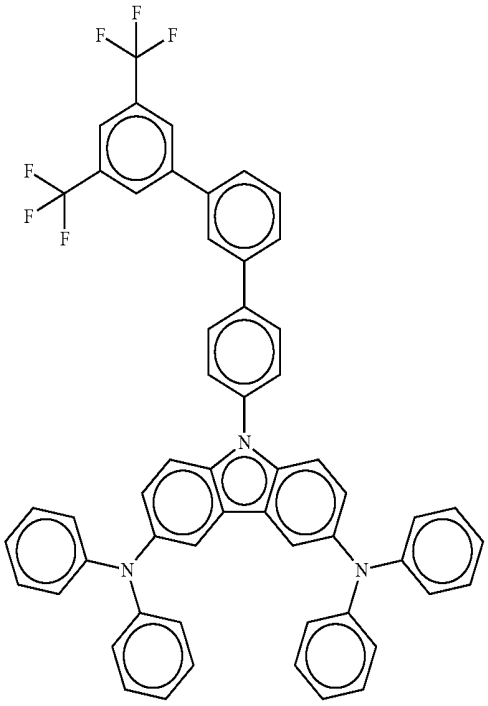


TABLE N-continued

N140



N141

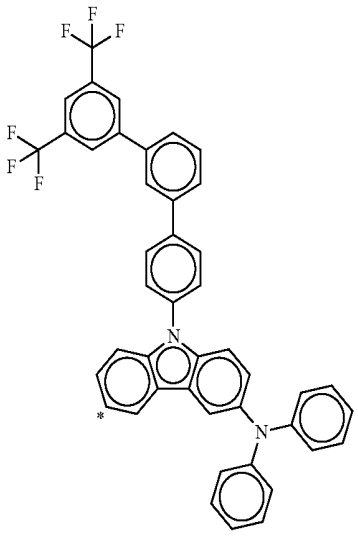
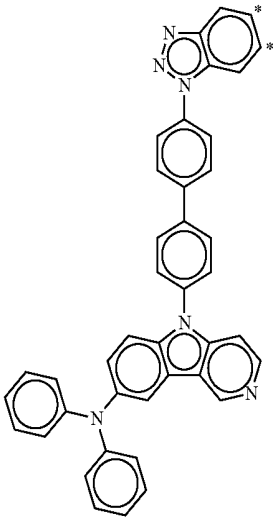
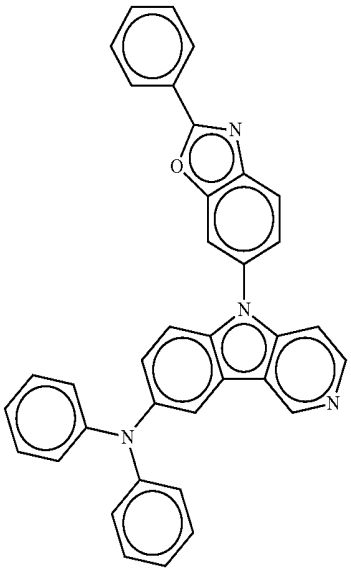


TABLE N-continued

N142



N143



N144

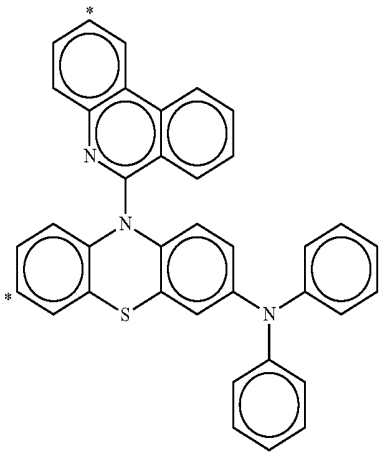
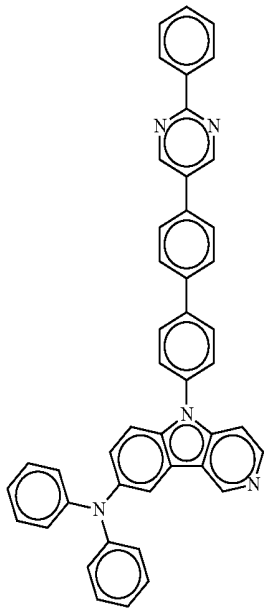
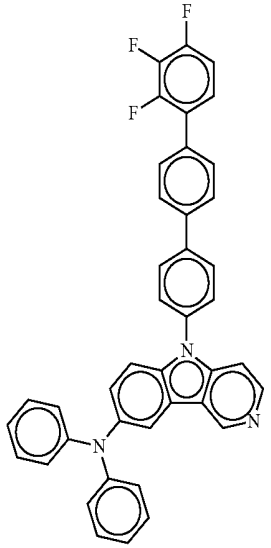


TABLE N-continued

N145



N146



N147

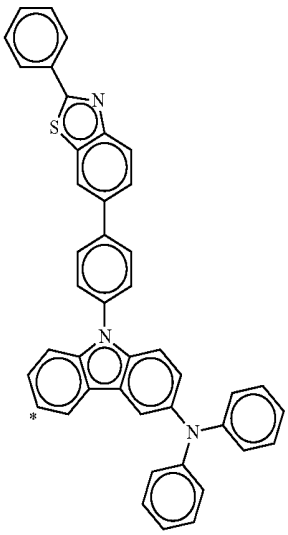
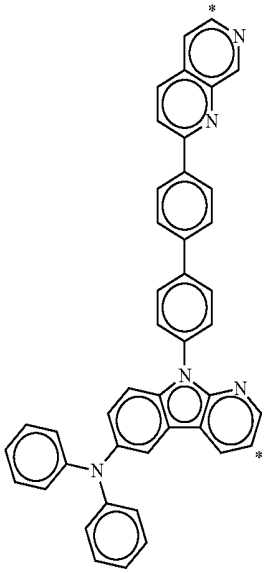


TABLE N-continued

N148



N149

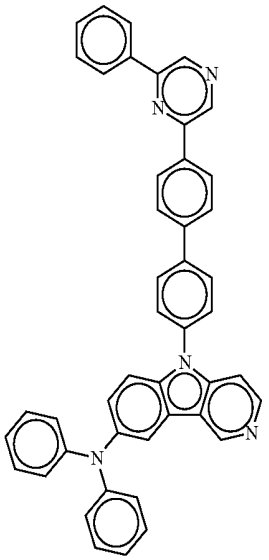
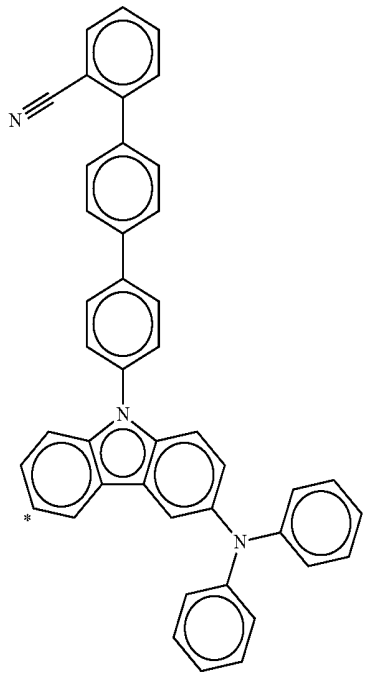
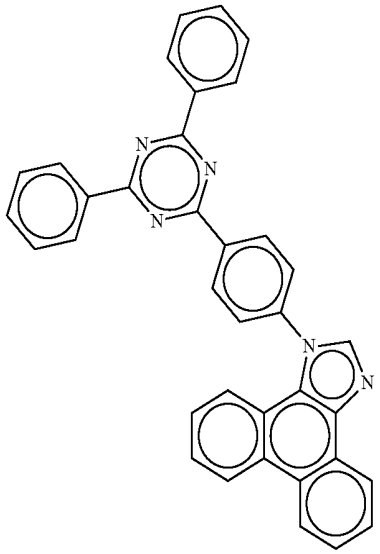


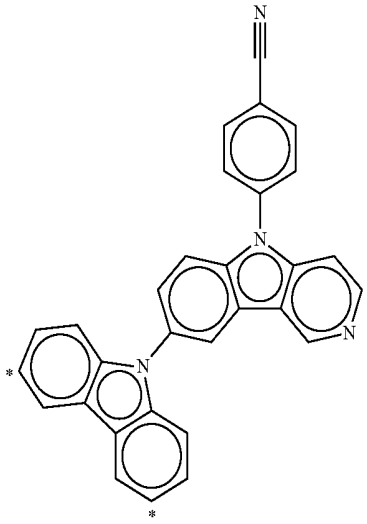
TABLE N-continued

N150	
N151	

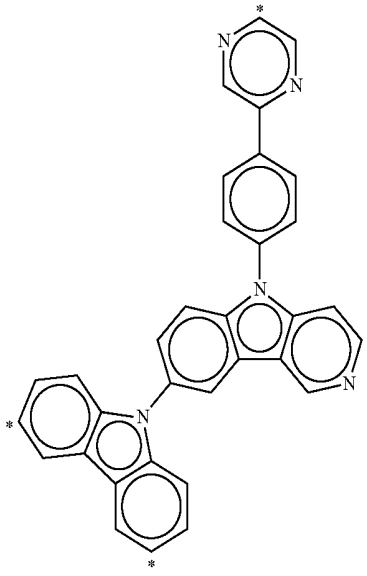
[0185] In example embodiments of the fourteenth aspect, the invention is any one compound selected from Table N'. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE N'

N44



N34



N59

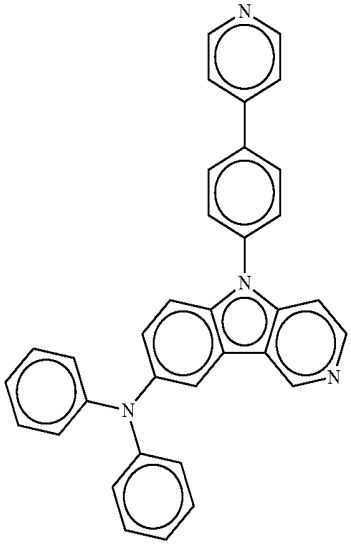
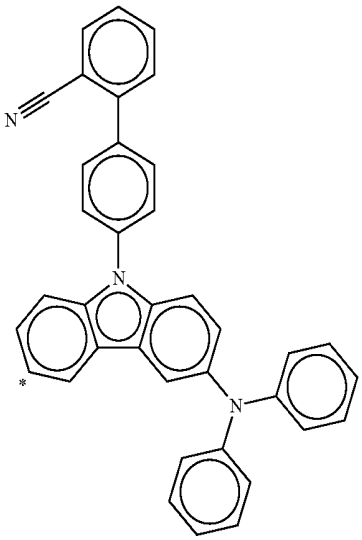


TABLE N'-continued

N17



N55

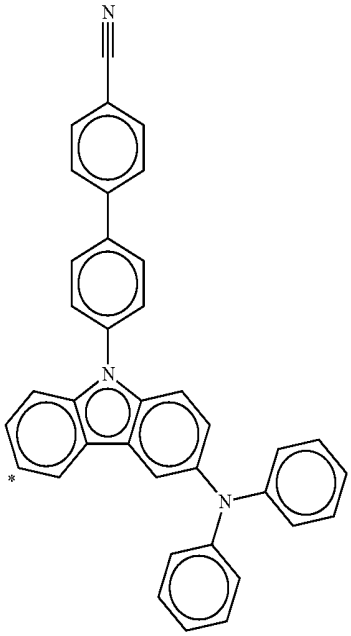


TABLE N'-continued

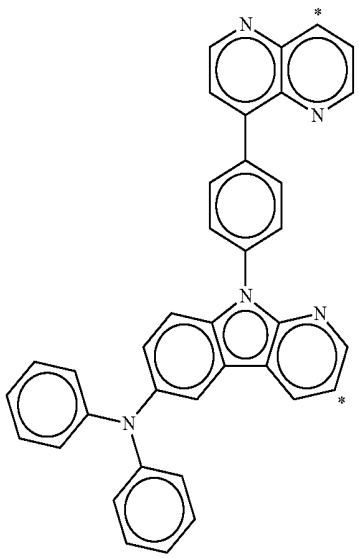
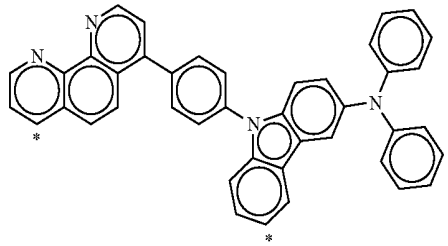
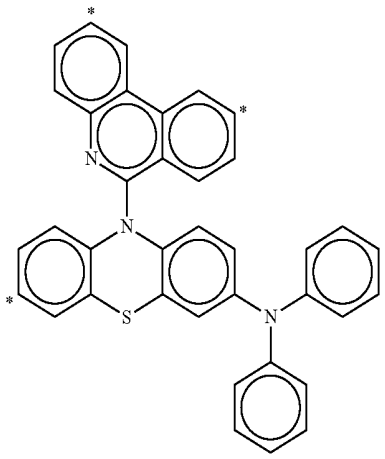
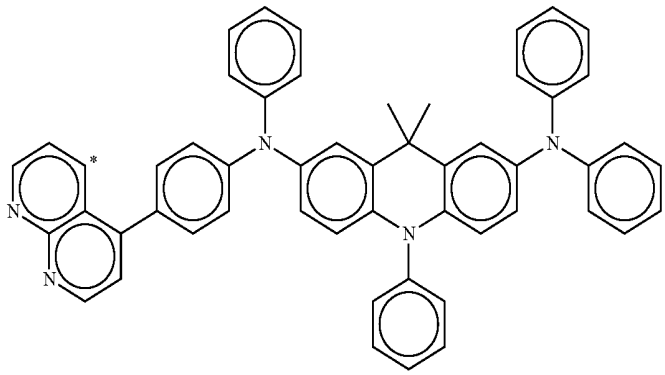
N14	

TABLE N'-continued

N68	

[0186] In example embodiments of the fourteenth aspect, the invention is any one compound selected from Table N". As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

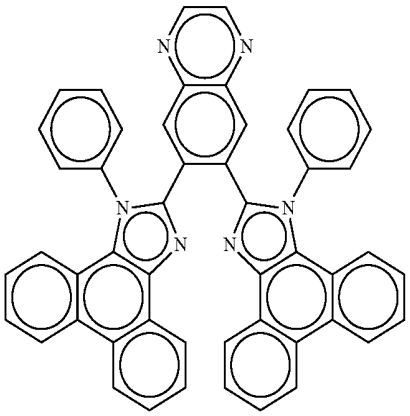
TABLE N"

N144	
N128	

[0187] In example embodiments of the fourteenth aspect, the invention is any one compound selected from Table N'''. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE N'''

N53



N92

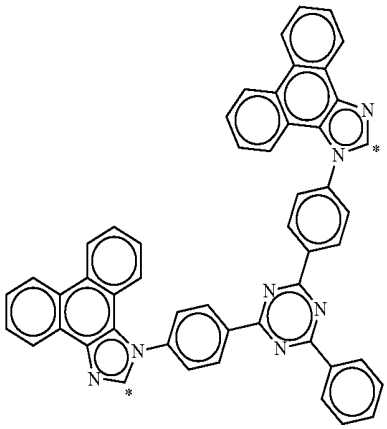
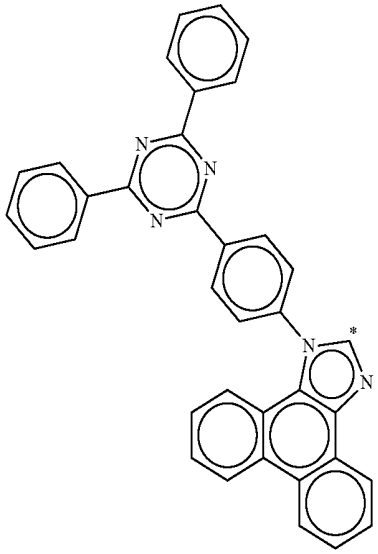


TABLE N'''-continued

N151



[0188] In example embodiments of the fourteenth aspect, the present invention is any one molecule selected from compounds O1 to O123, listed in Table O. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE O

O1

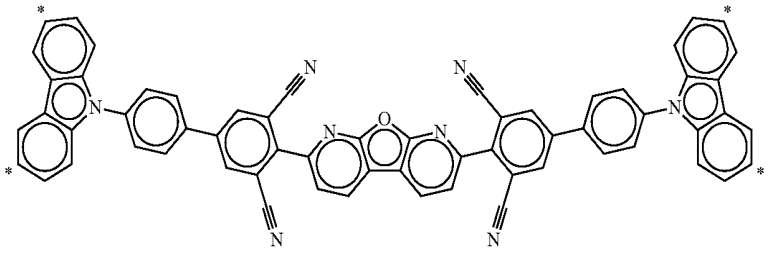


TABLE O-continued

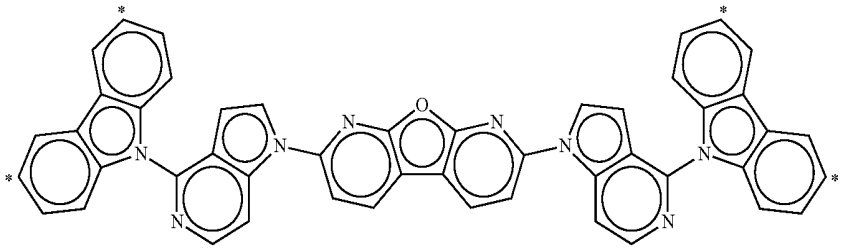
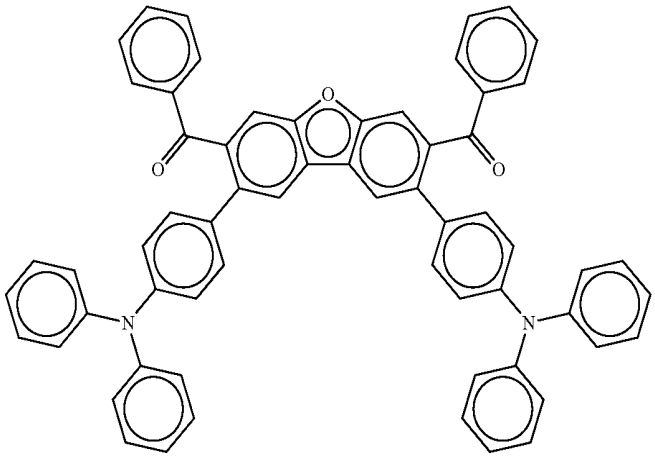
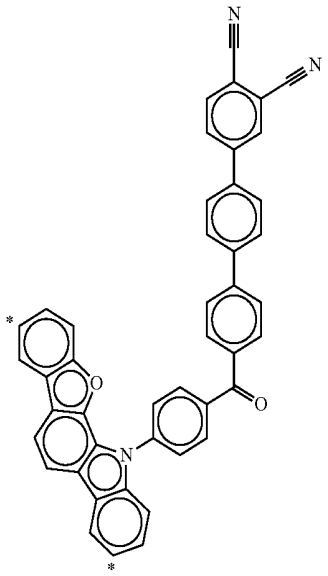
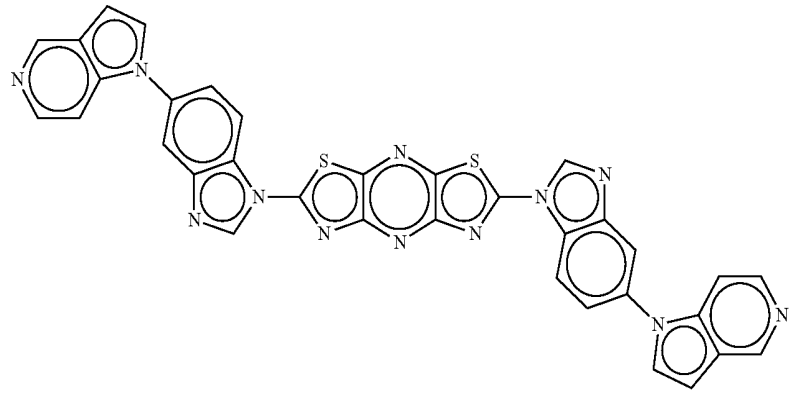
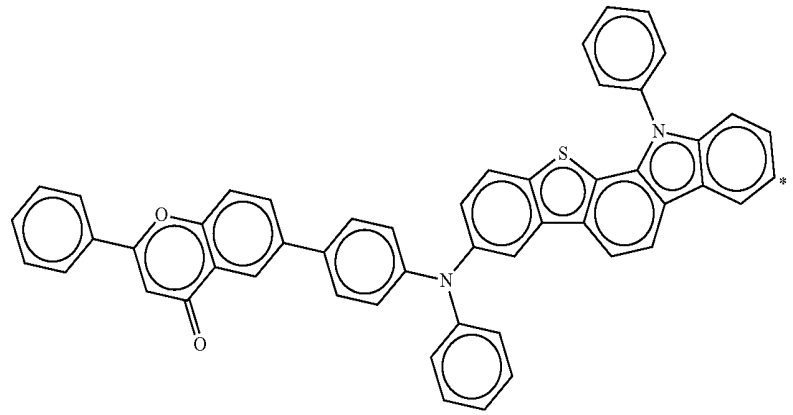
	O2
	O3
	O4

TABLE O-continued

O5



O6



O7

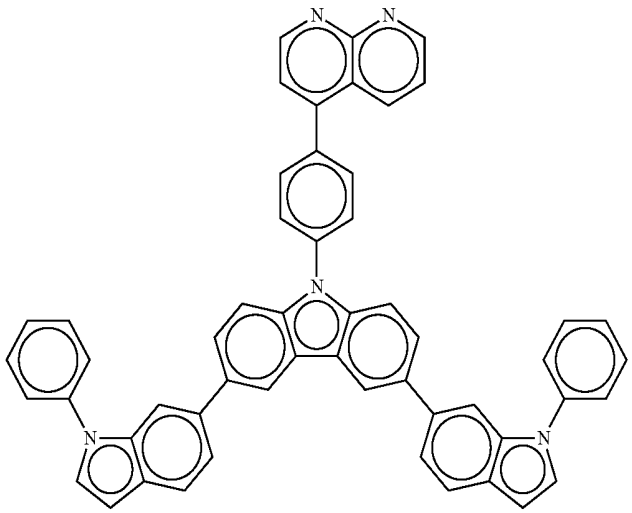
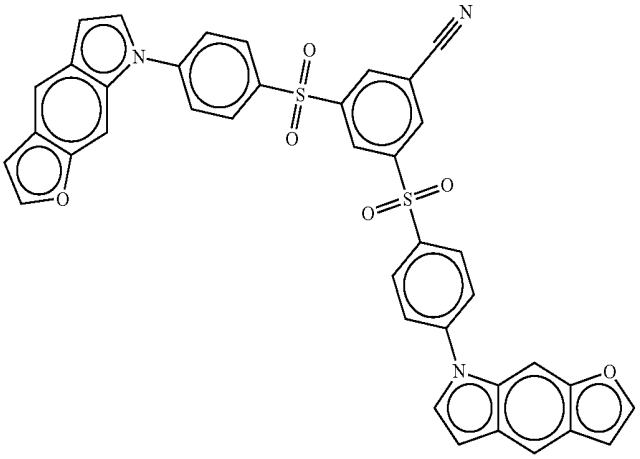
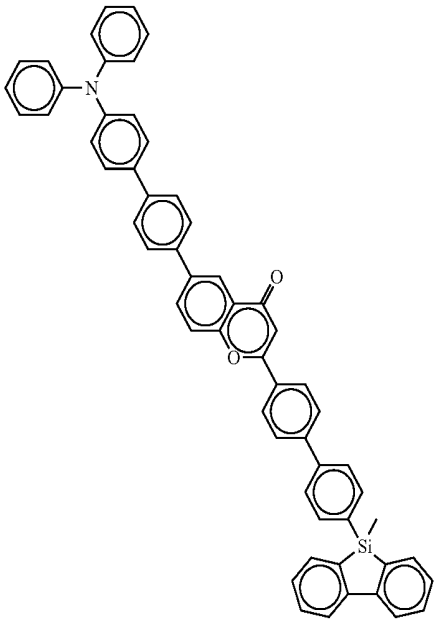


TABLE O-continued

O8



O9



O10

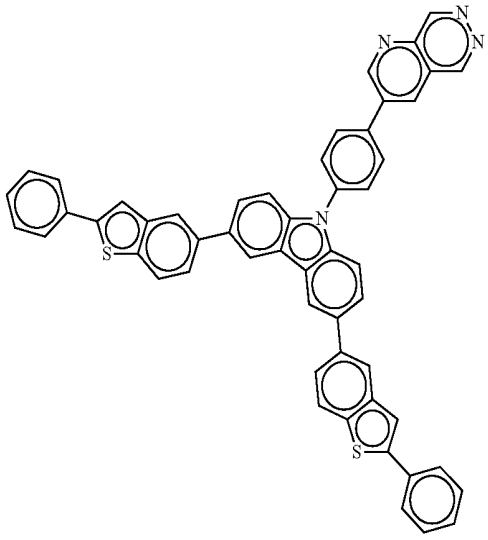
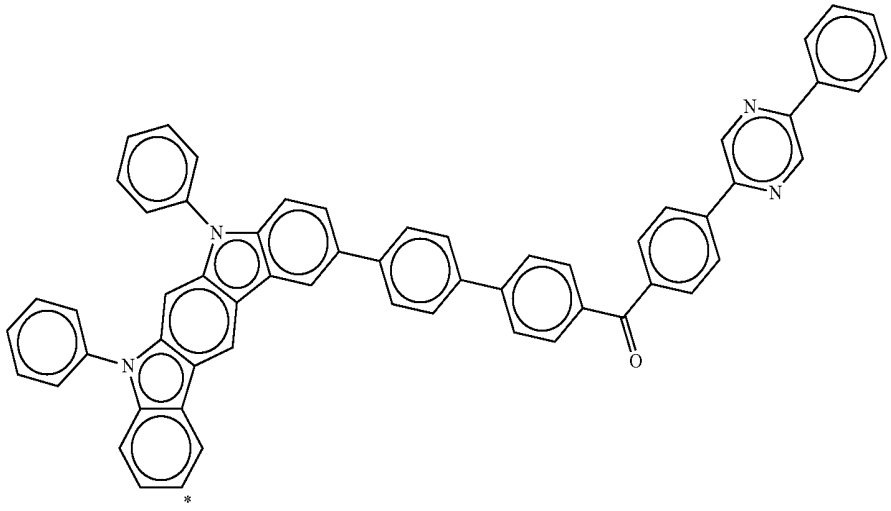


TABLE O-continued

O11



O12

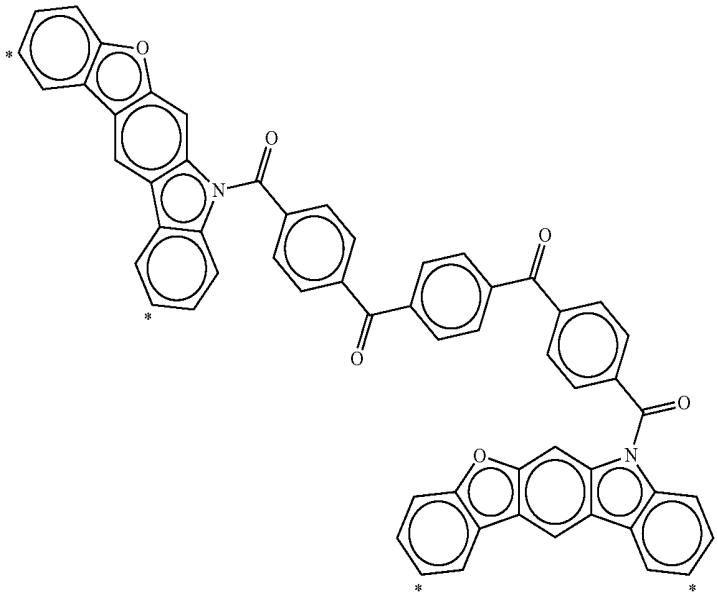
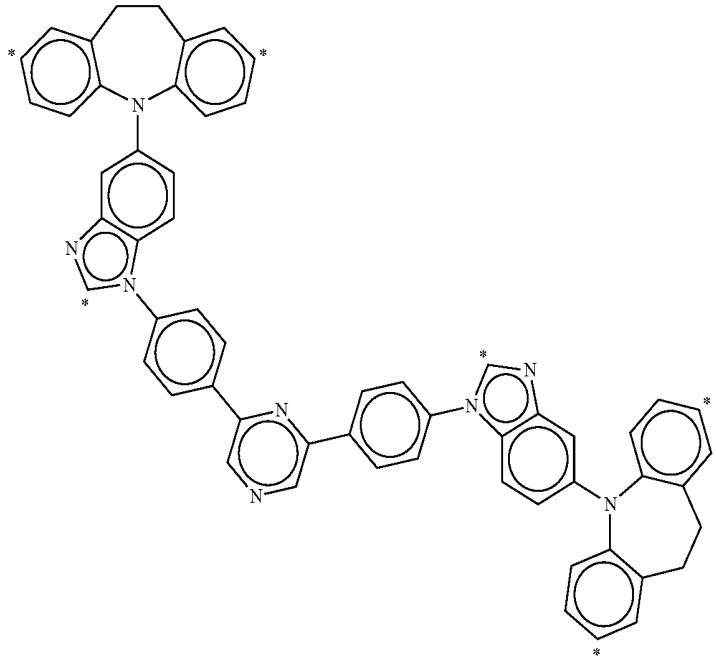


TABLE O-continued

O13



O14

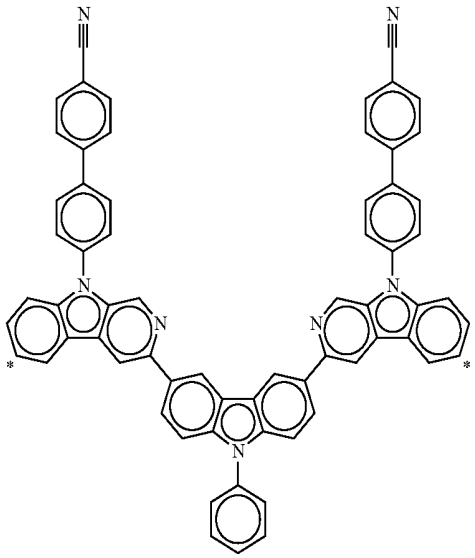
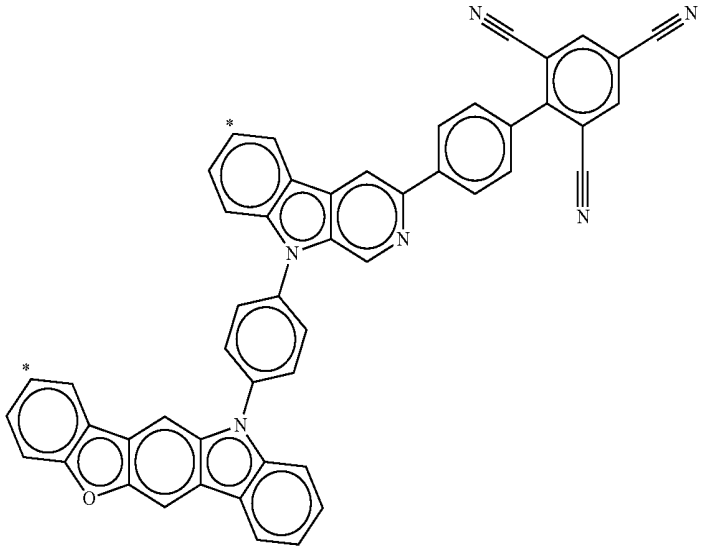
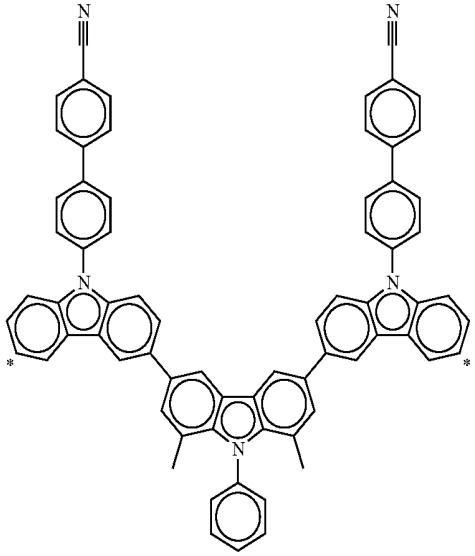


TABLE O-continued

O15



O16



O17

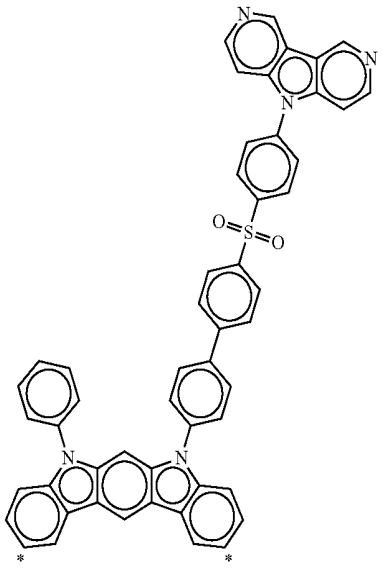


TABLE O-continued

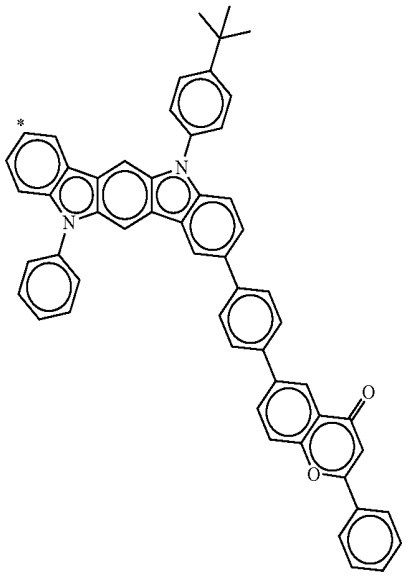
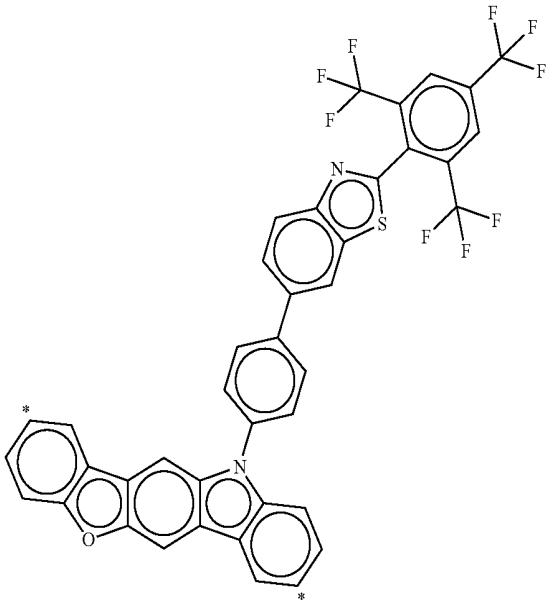
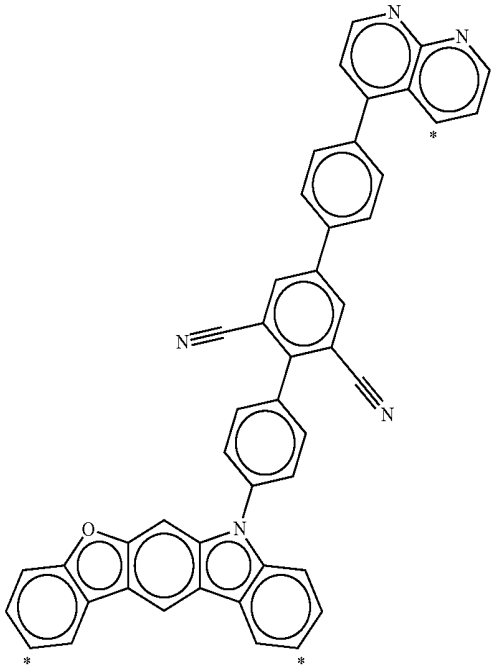
O18	
O19	

TABLE O-continued

O20



O21

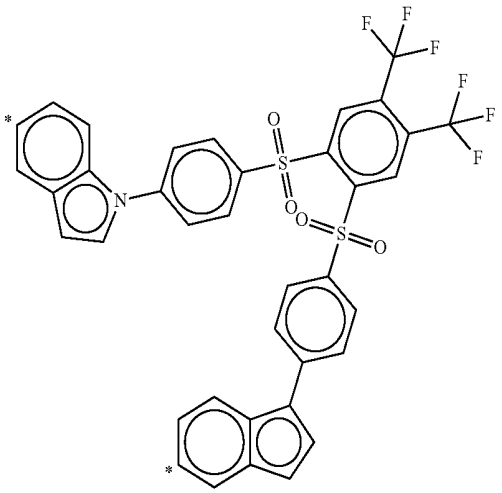
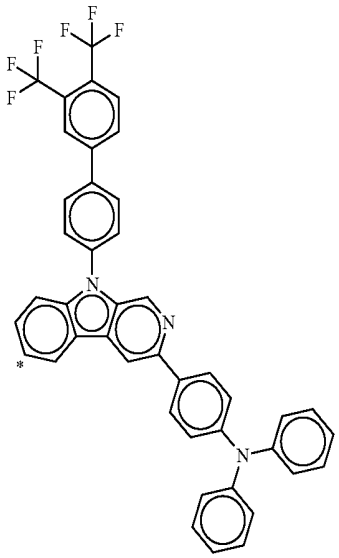
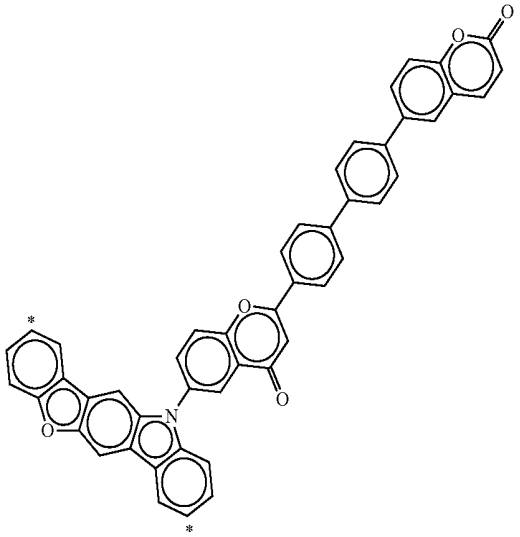


TABLE O-continued

O22



O23



O24

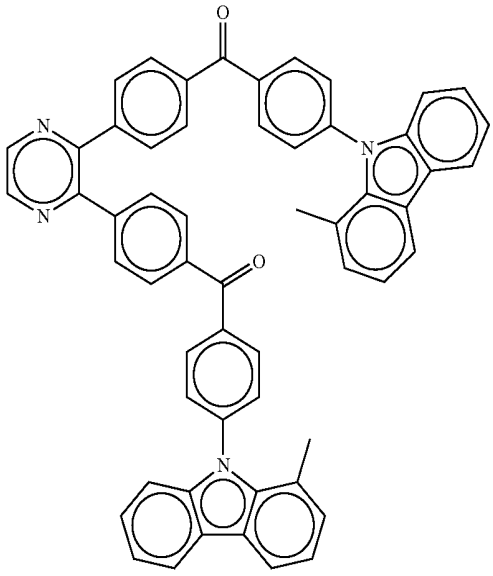
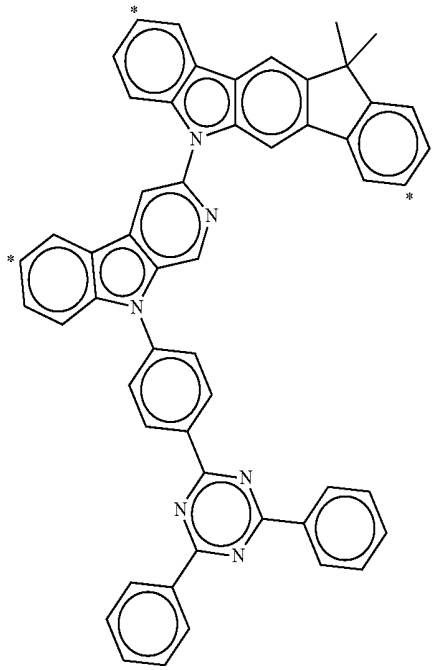


TABLE O-continued

O25



O26

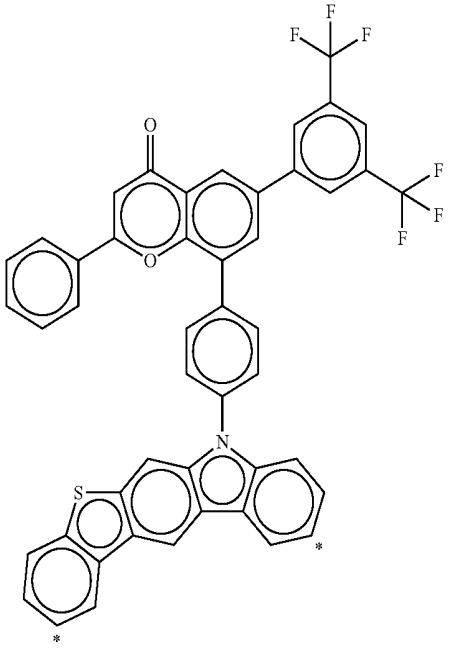
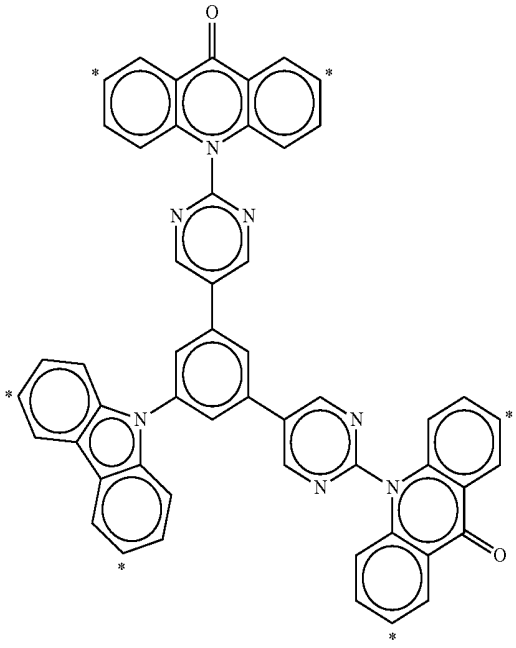


TABLE O-continued

O27



O28

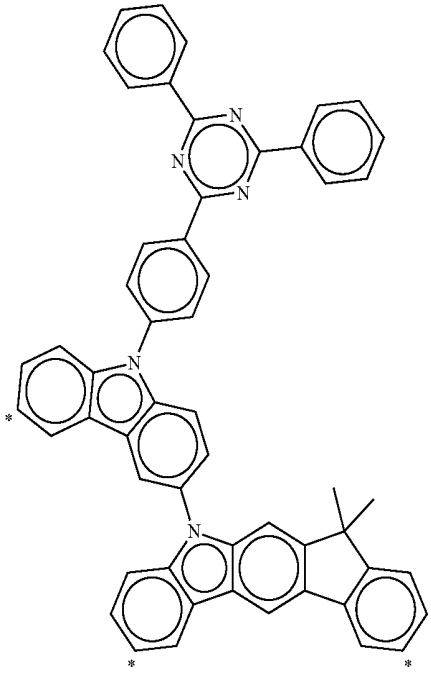
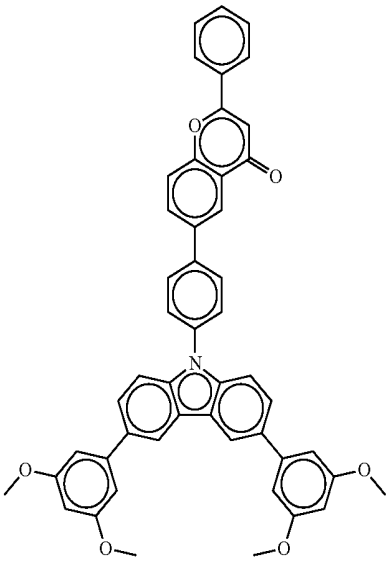
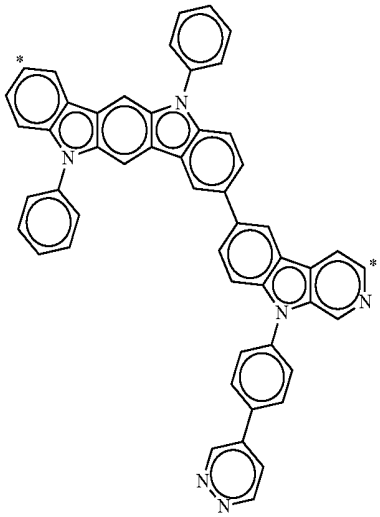


TABLE O-continued

O29



O30



O31

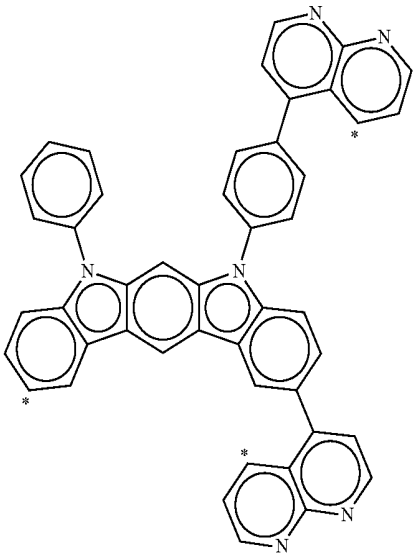
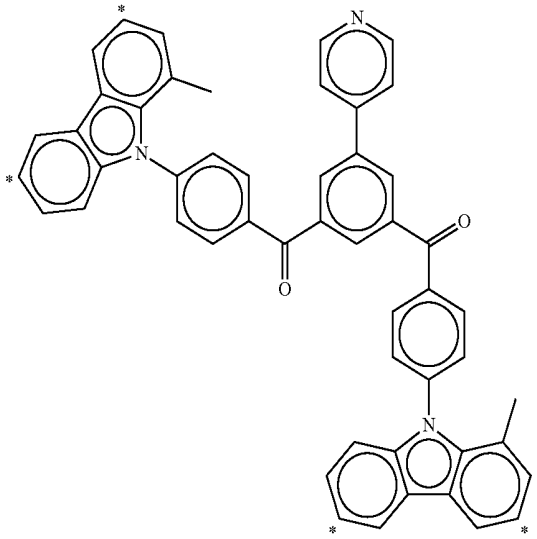
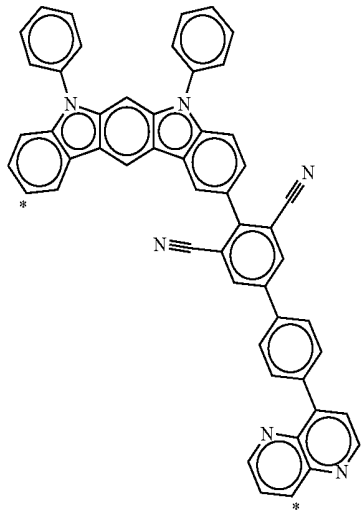


TABLE O-continued

O32



O33



O34

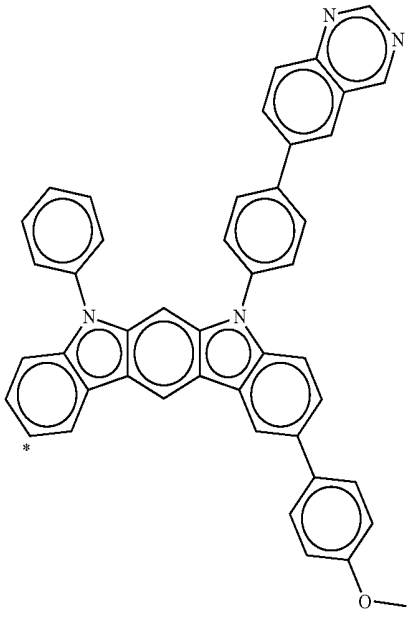
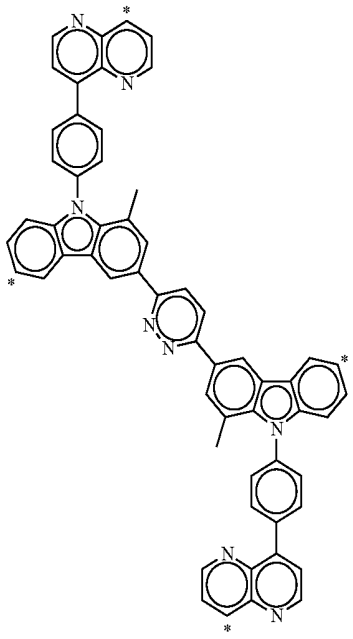


TABLE O-continued

O35



O36

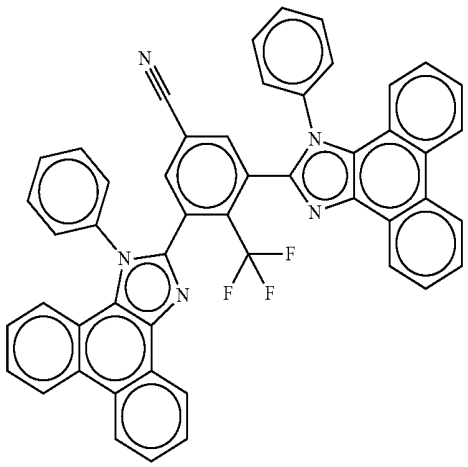
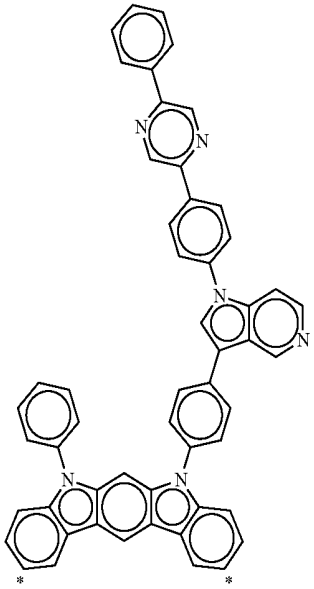


TABLE O-continued

O37



O38

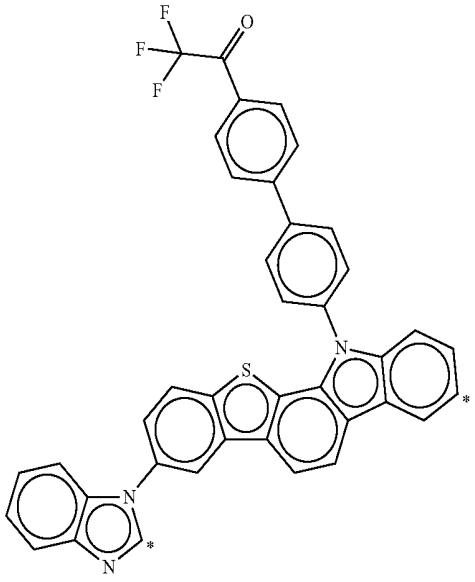
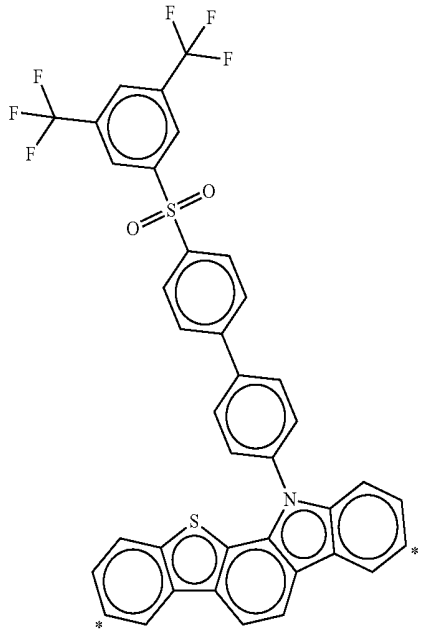


TABLE O-continued

O39



O40

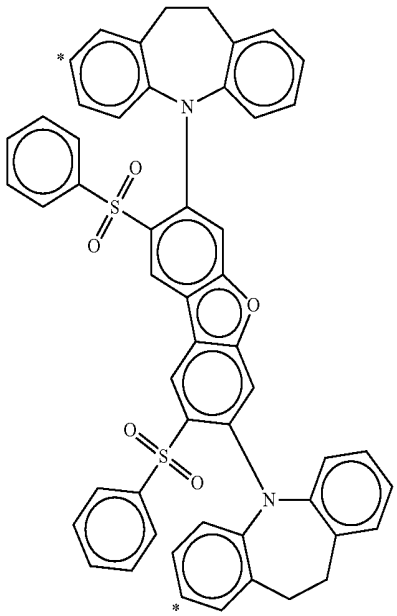
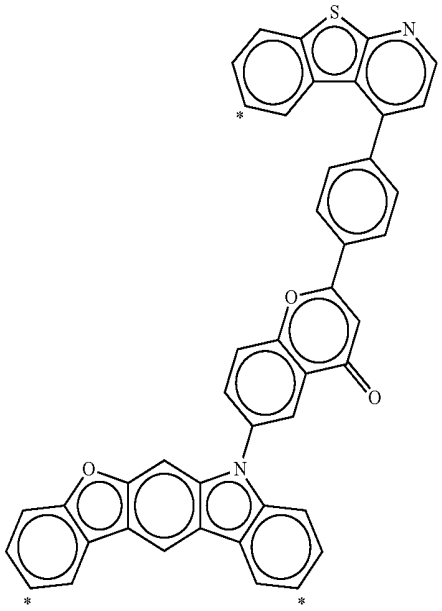


TABLE O-continued

O41



O42

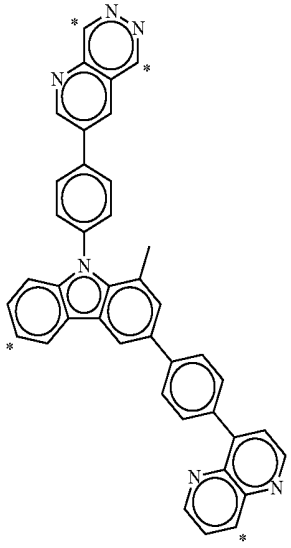
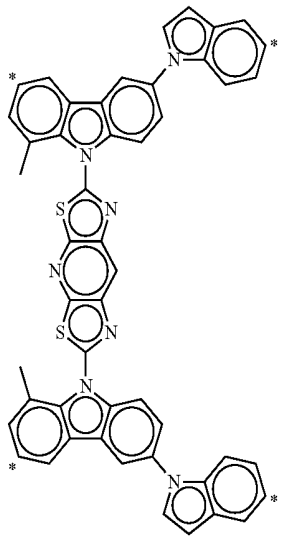
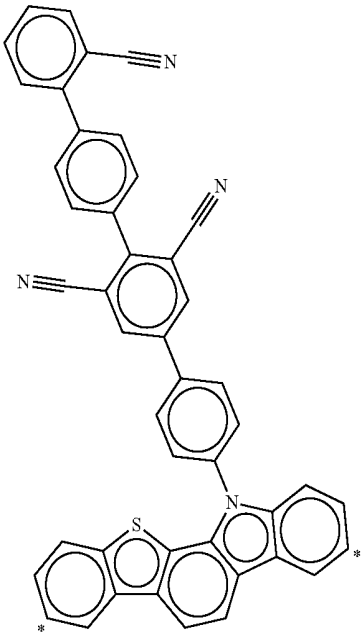


TABLE O-continued

O43



O44



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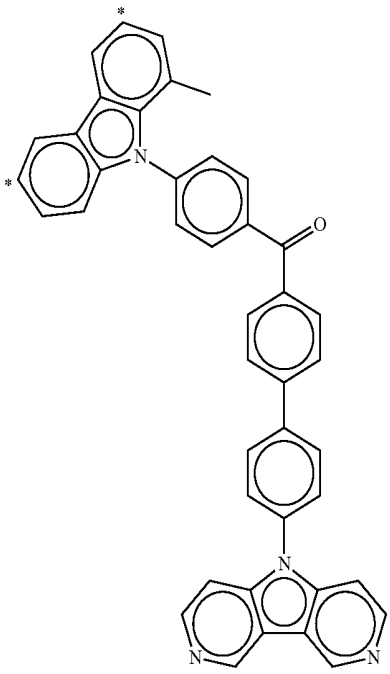
O45



O46

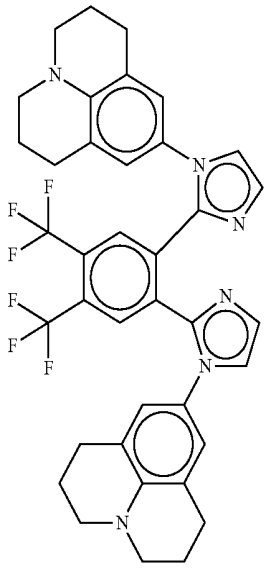
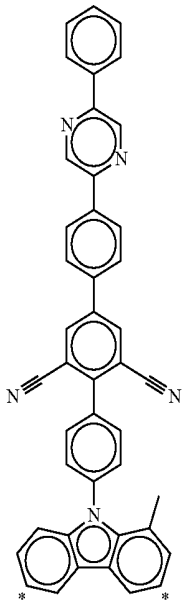


TABLE O-continued

O47



O48

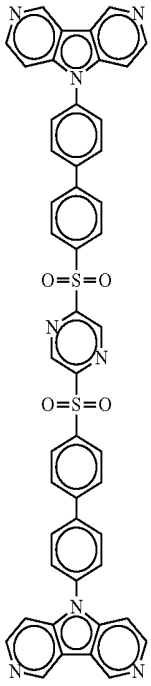
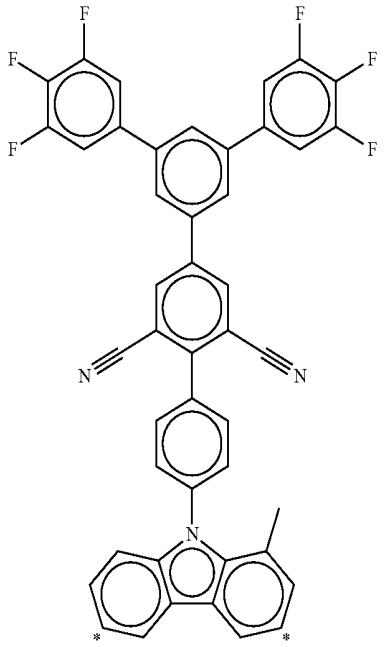


TABLE O-continued

O49



O50

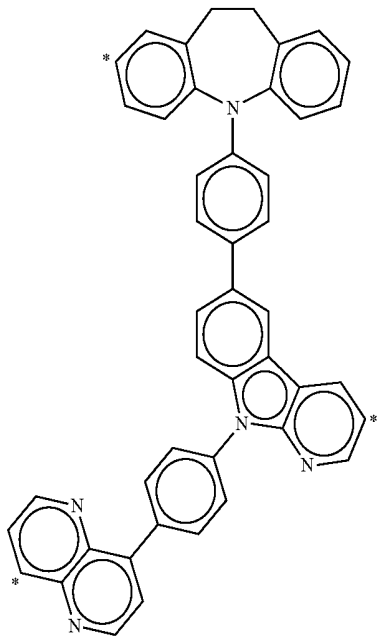
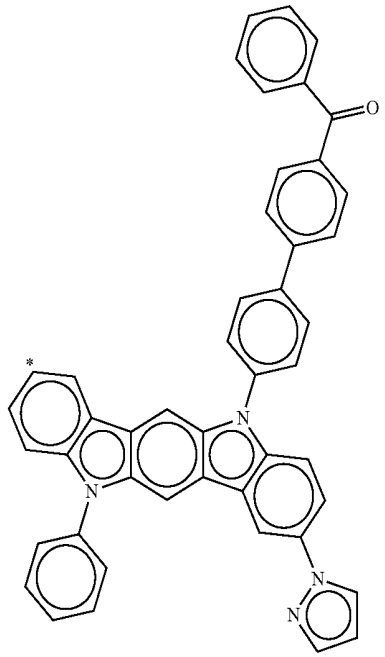
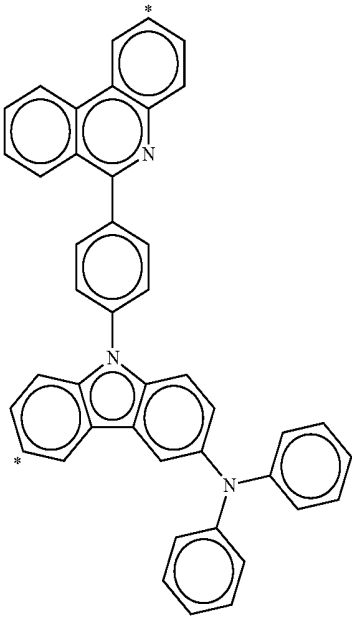


TABLE O-continued

O51



O52



O53

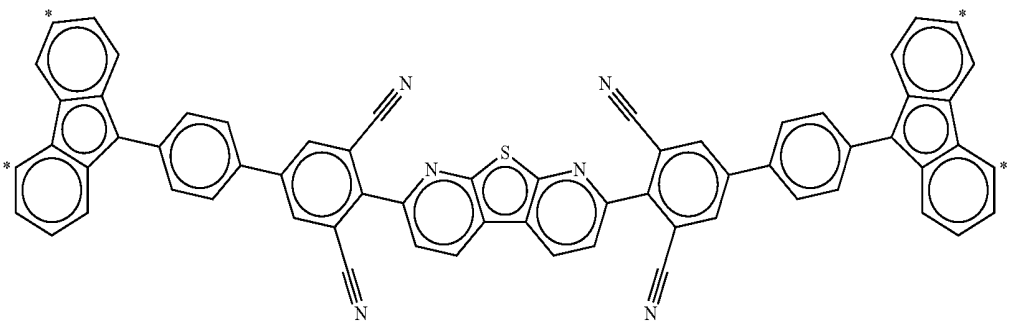
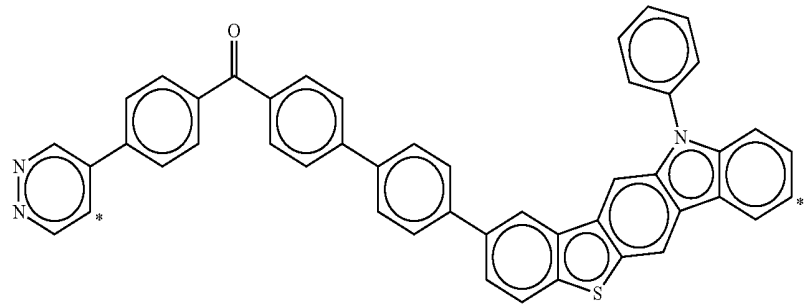
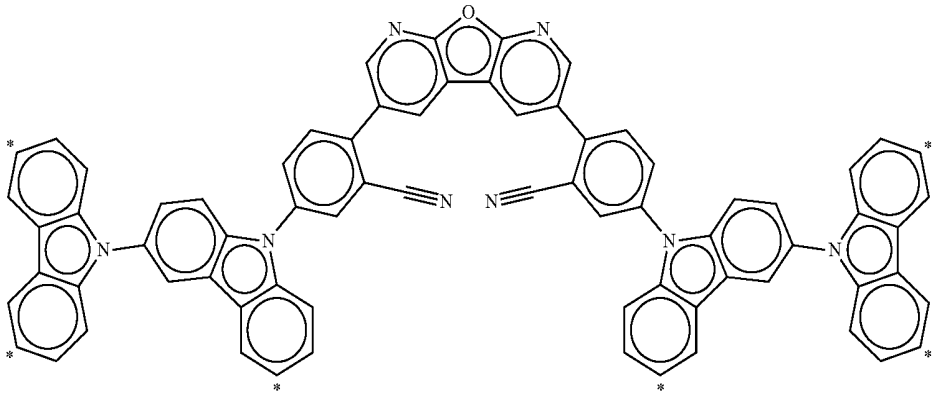


TABLE O-continued

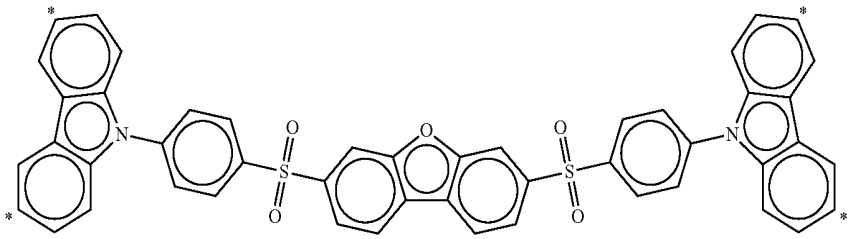
O54



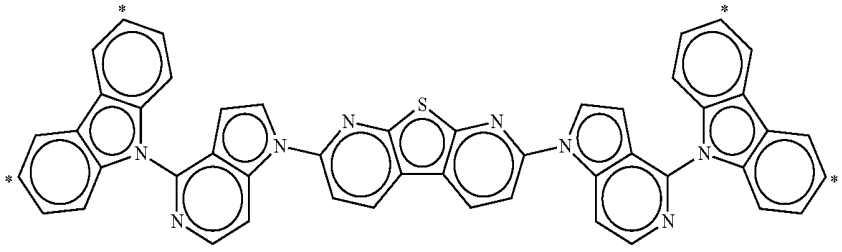
O55



O56



O57



O58

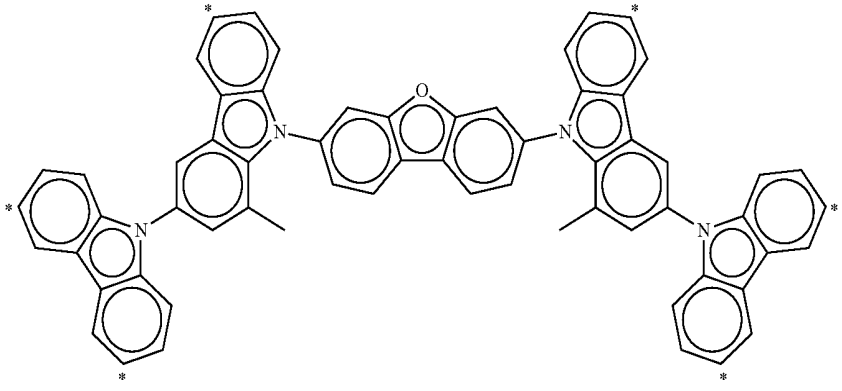
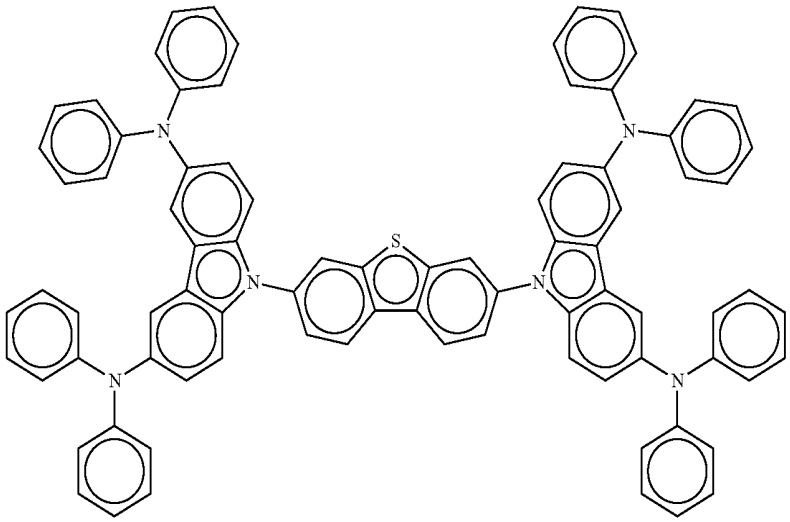


TABLE O-continued

O59



O60

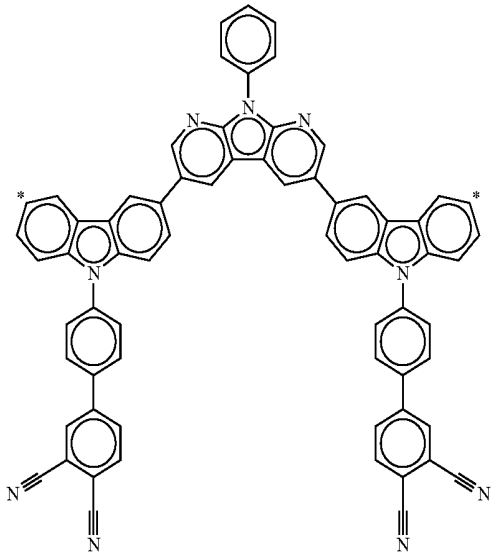
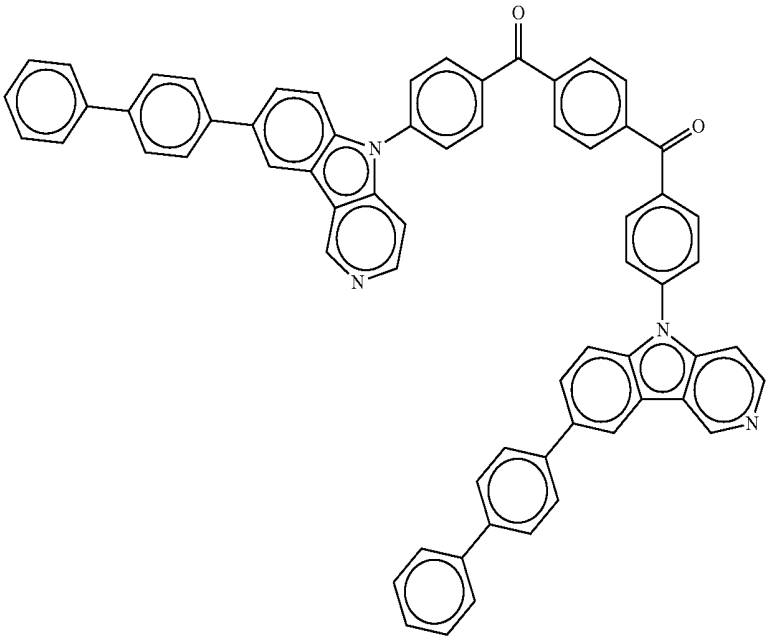


TABLE O-continued

O61



O62

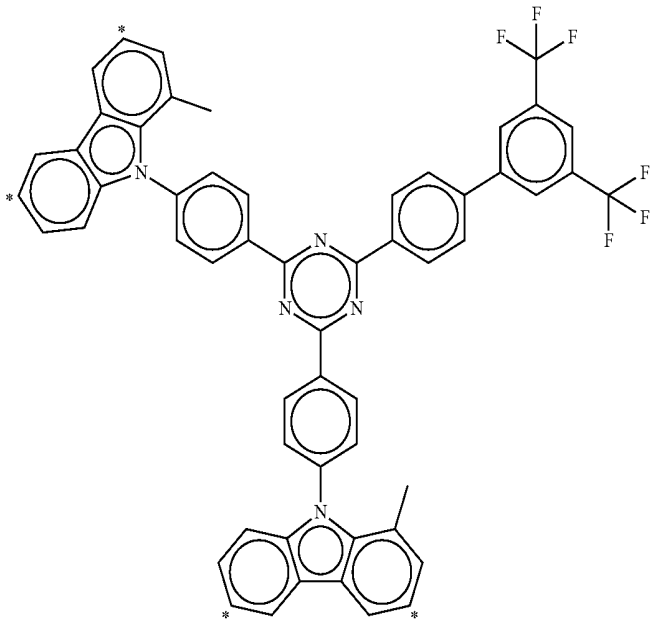
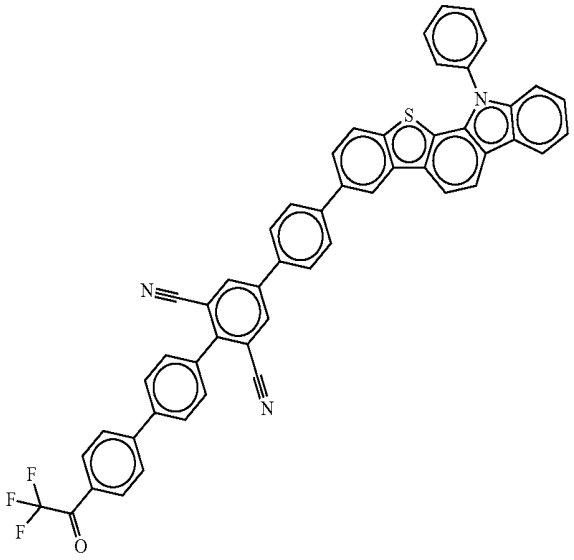


TABLE O-continued

O63



O64

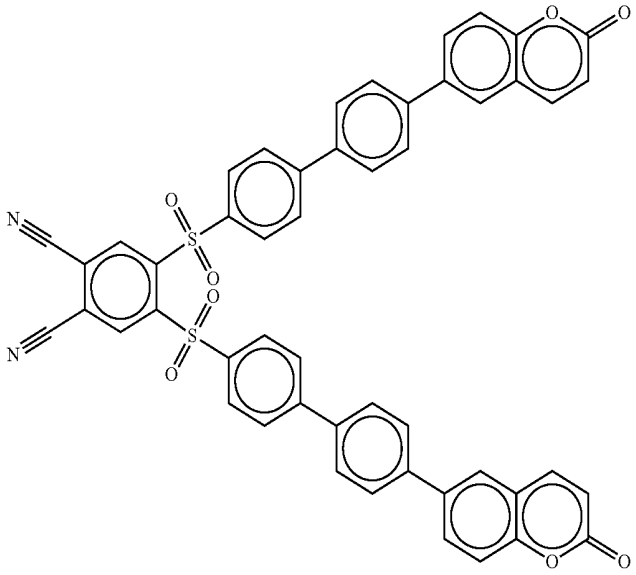
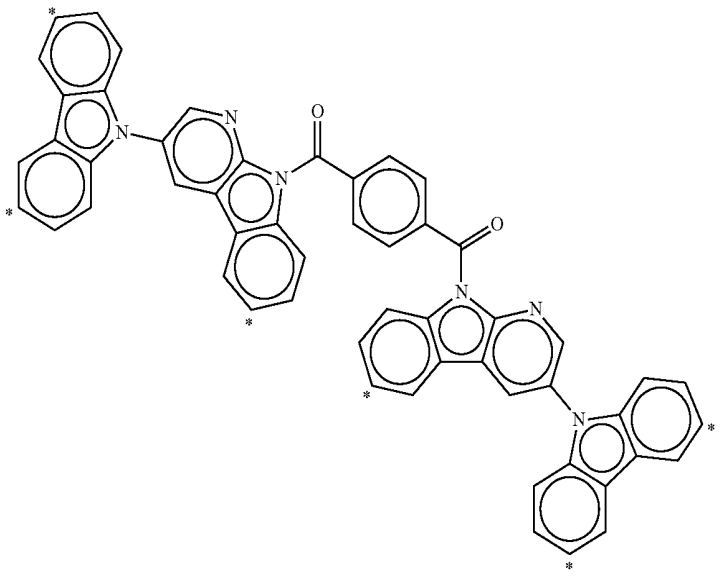


TABLE O-continued

O65



O66

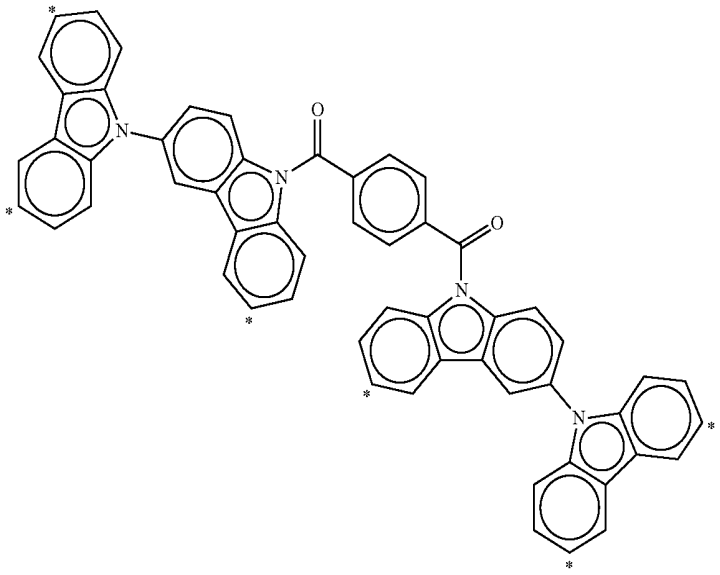
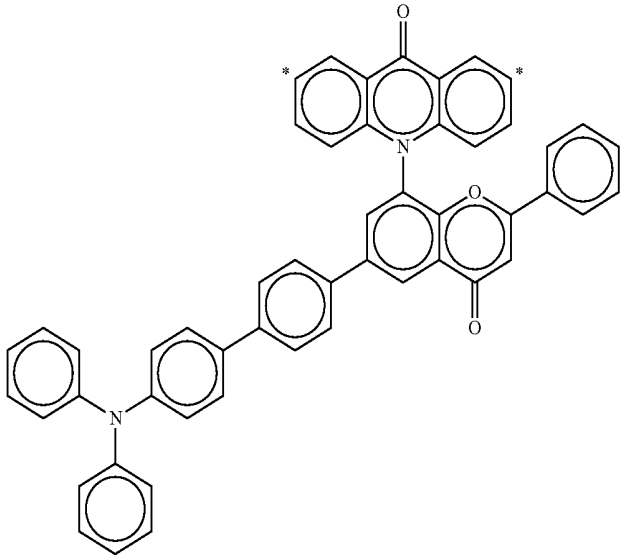


TABLE O-continued

O67



O68

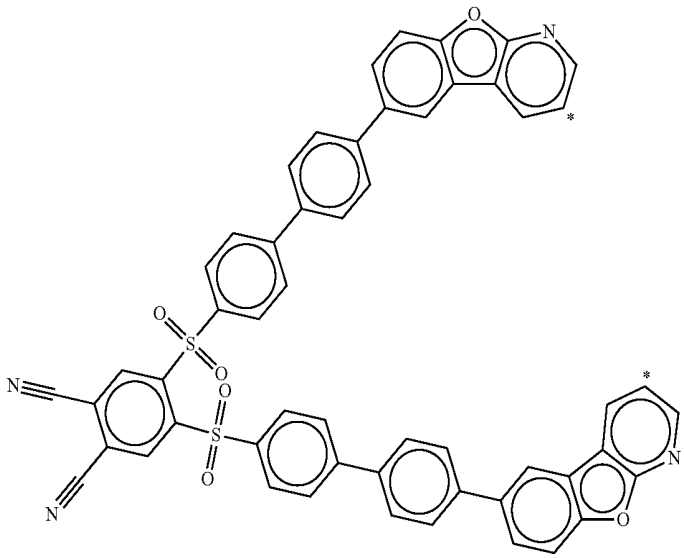
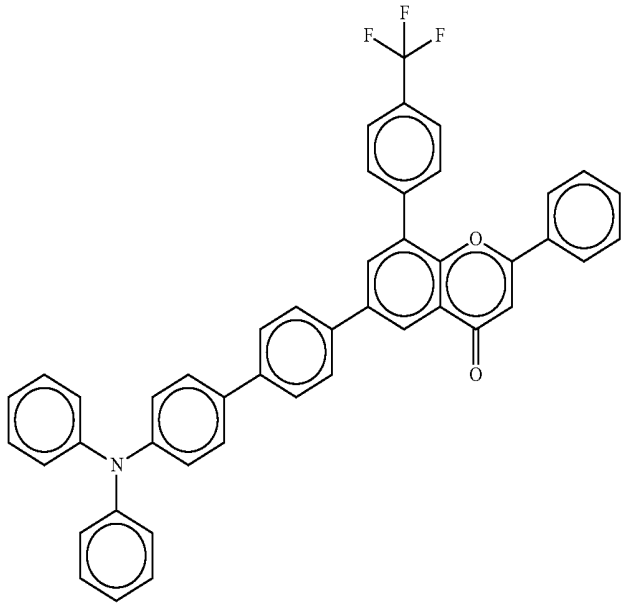
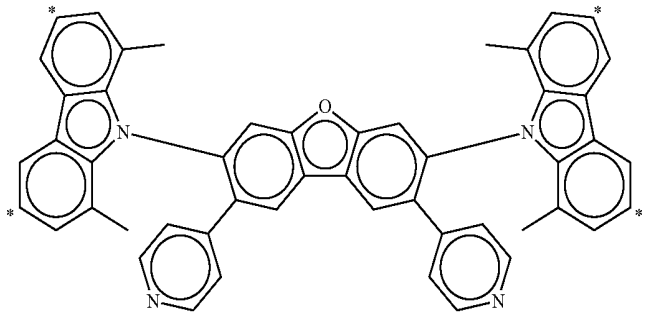


TABLE O-continued

O69



O70



O71

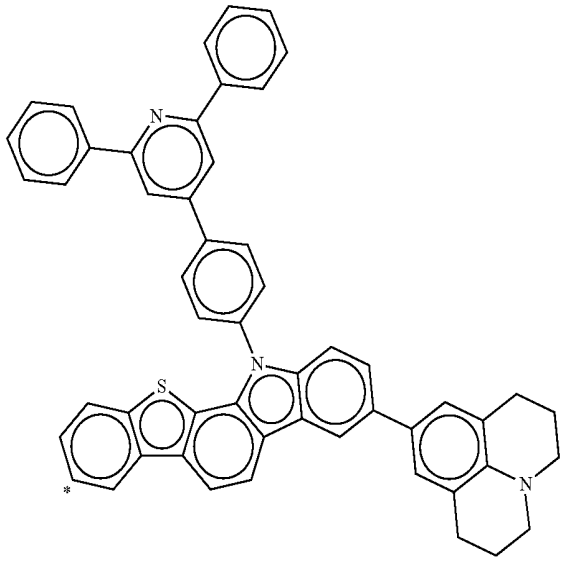
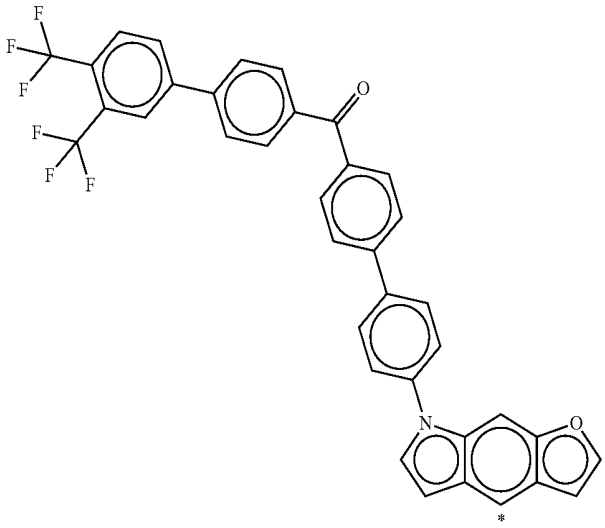
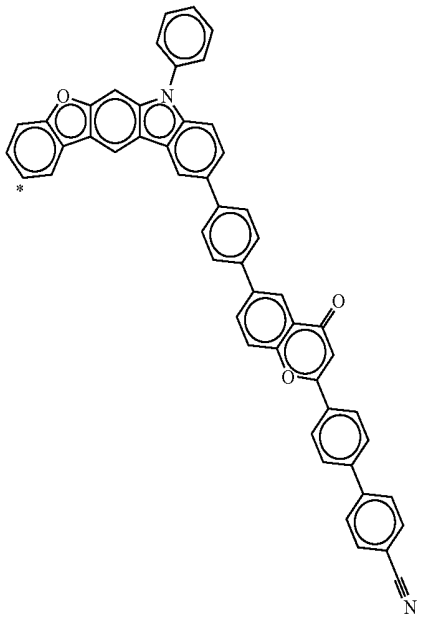


TABLE O-continued

O72



O73



O74

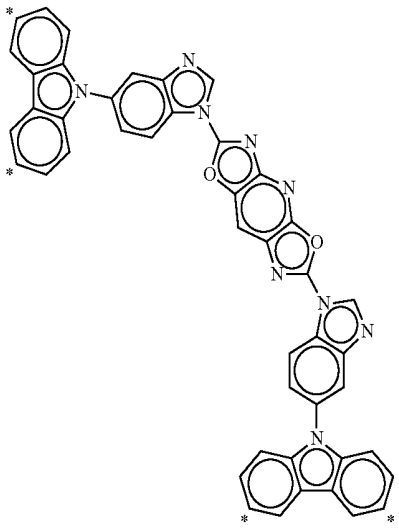
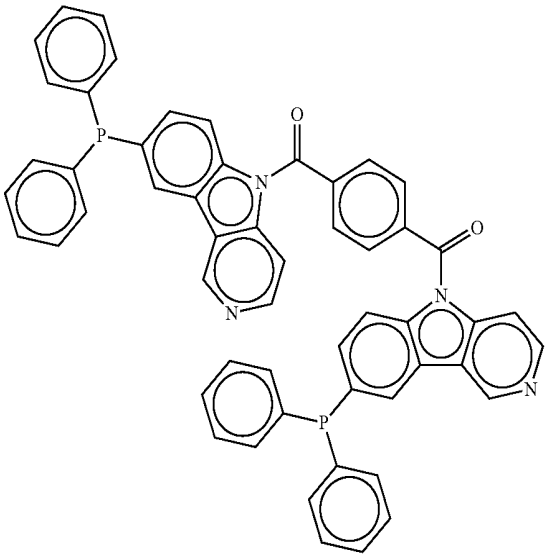
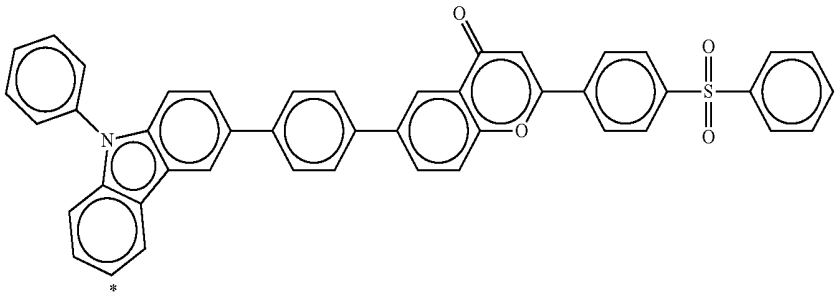


TABLE O-continued

O75



O76



O77

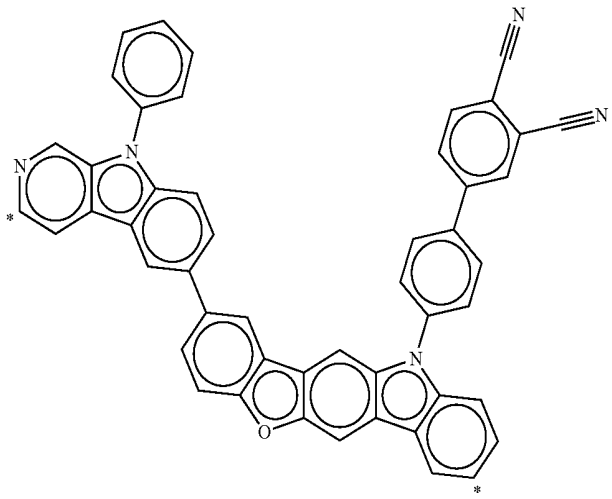
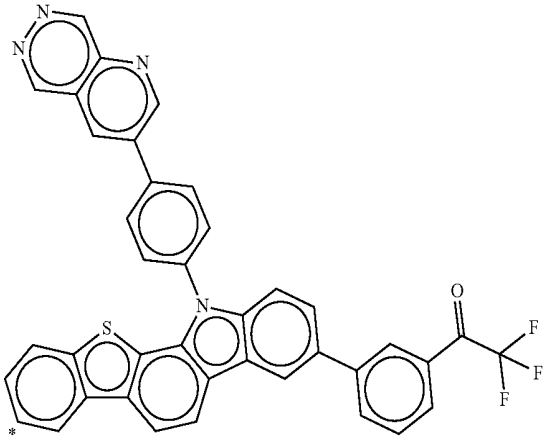
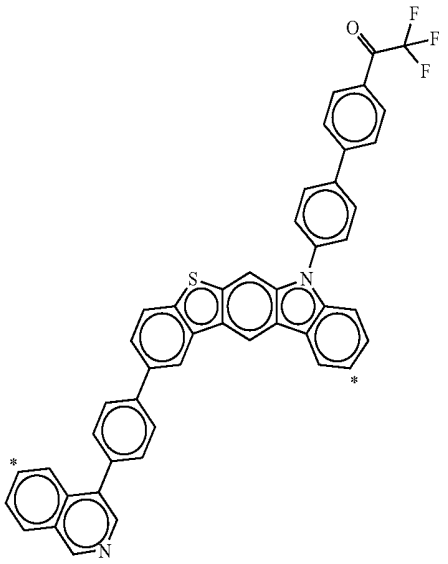


TABLE O-continued

O78



O79



O80

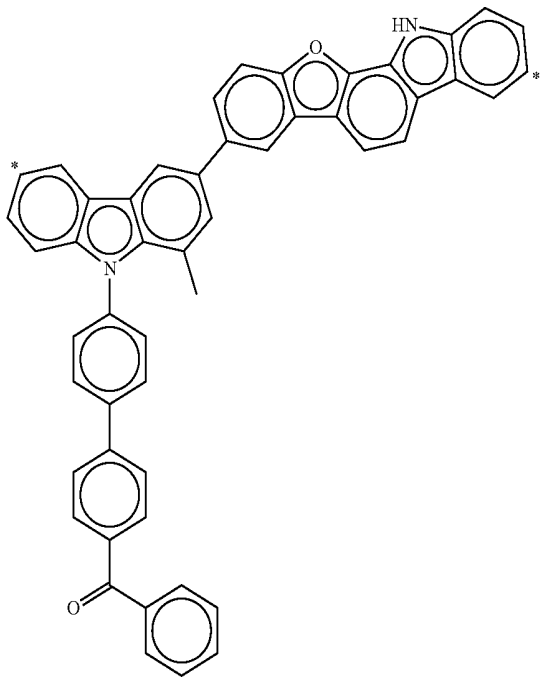
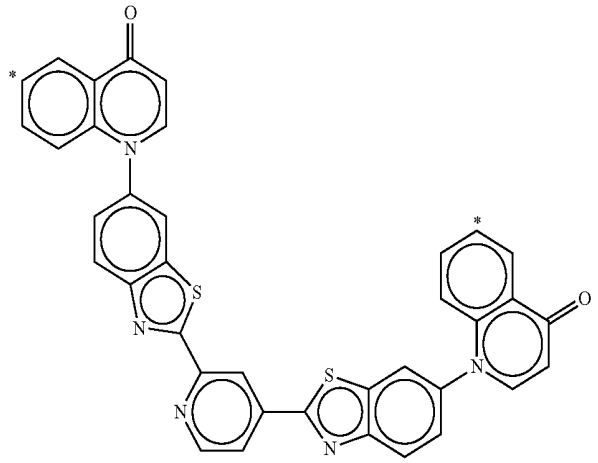
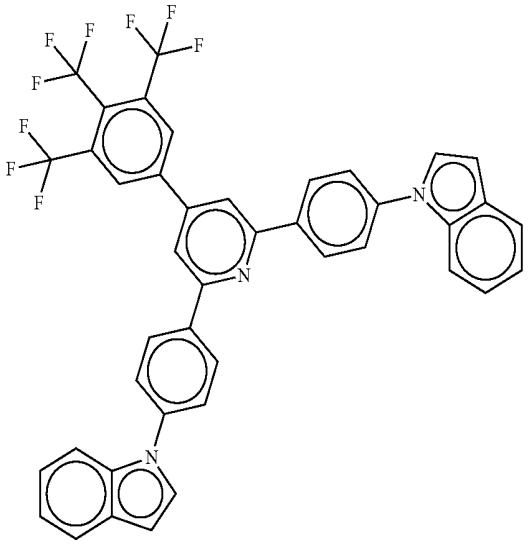


TABLE O-continued

O81



O82



O83

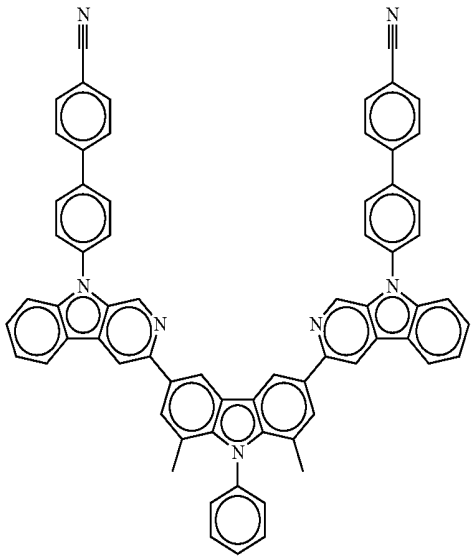
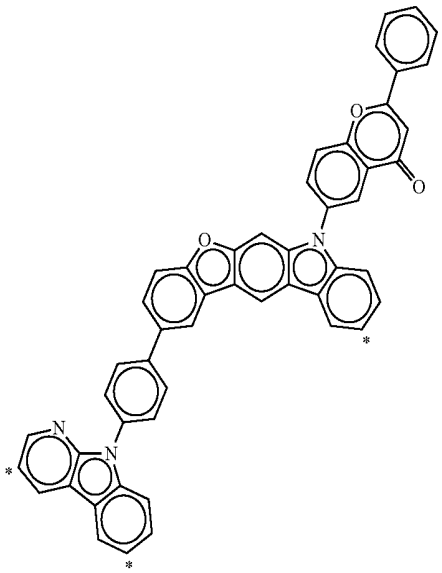
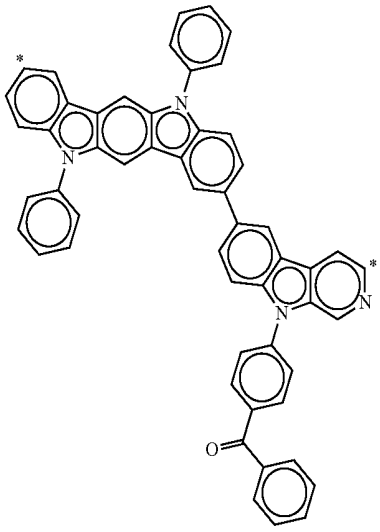


TABLE O-continued

O84



O85



O86

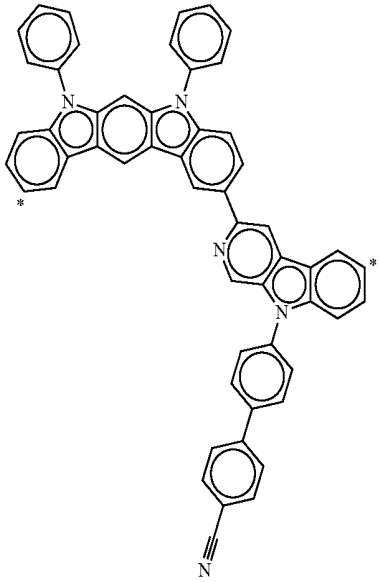
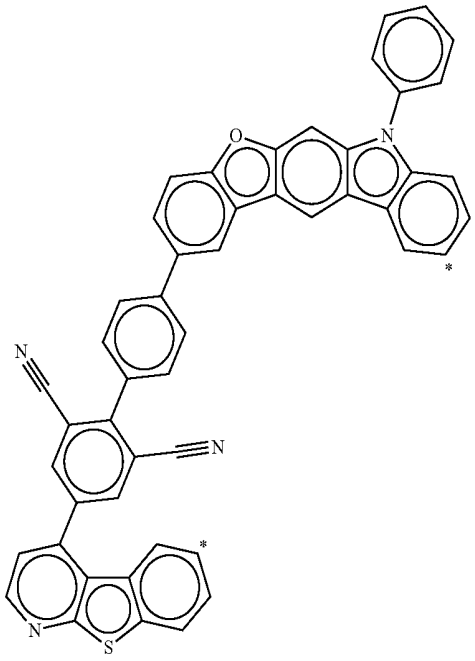


TABLE O-continued

O87



O88

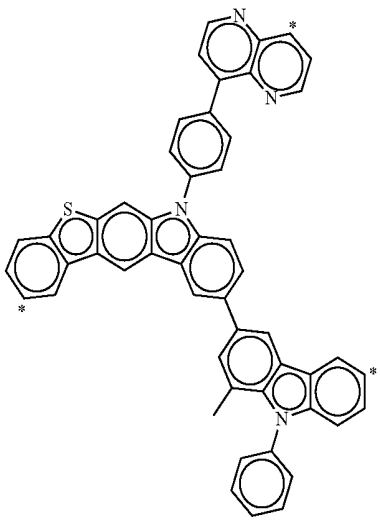
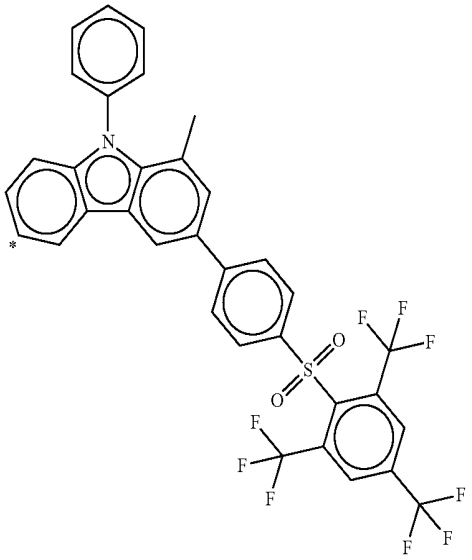


TABLE O-continued

O89



O90

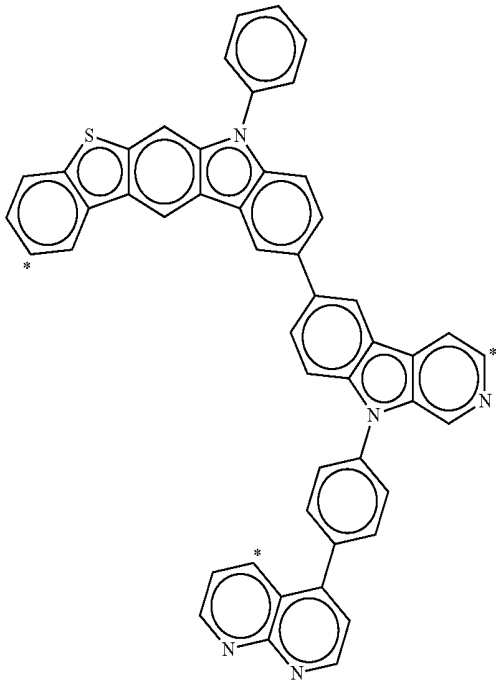
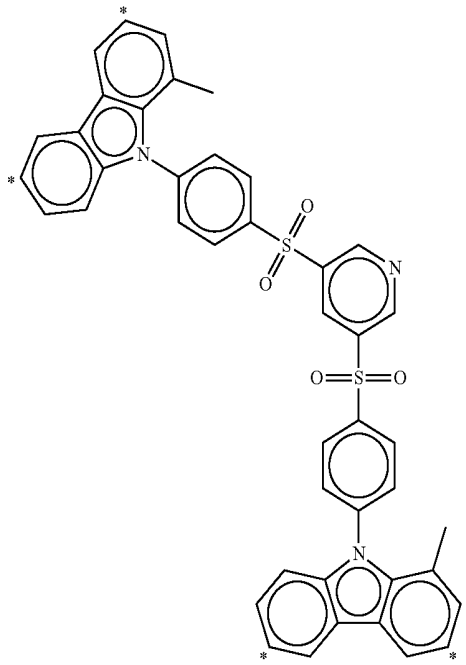


TABLE O-continued

O91



O92

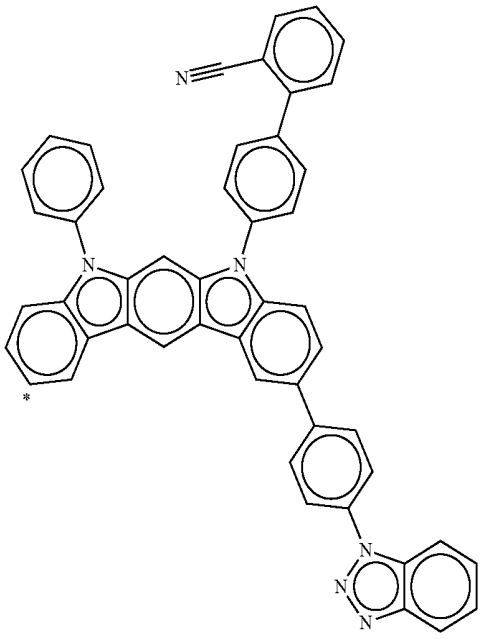
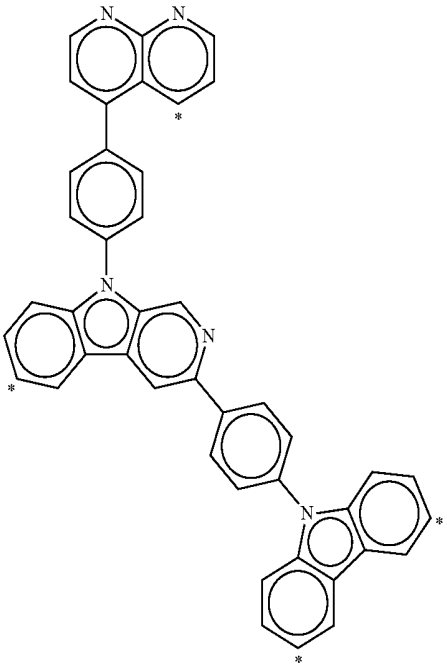


TABLE O-continued

O93



O94

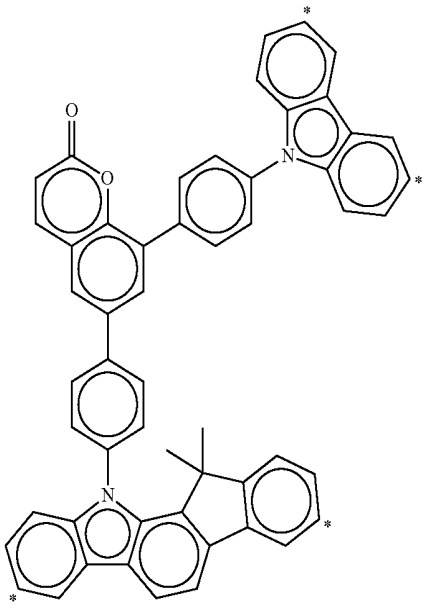
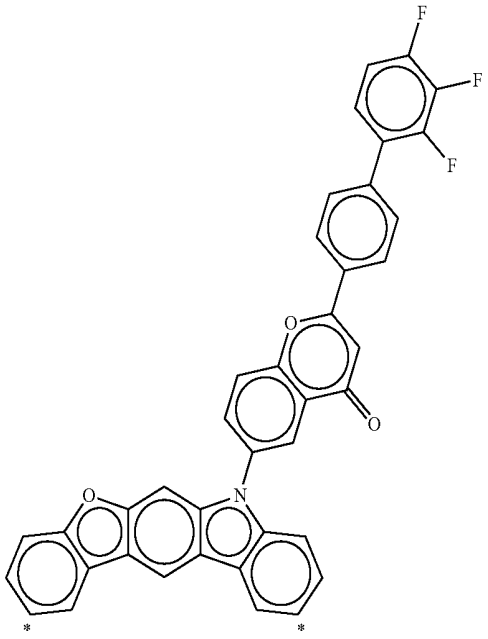


TABLE O-continued

O95



O96

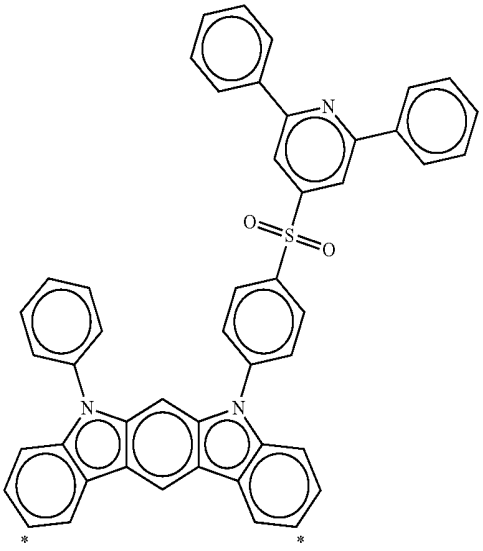
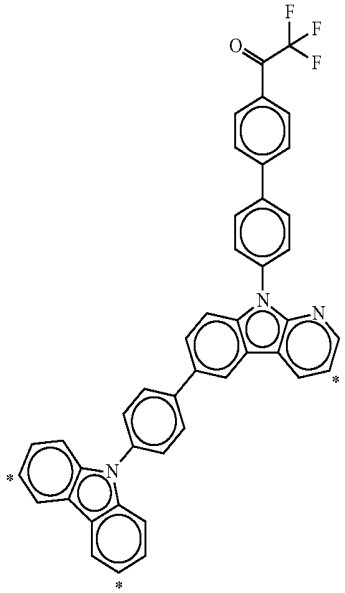
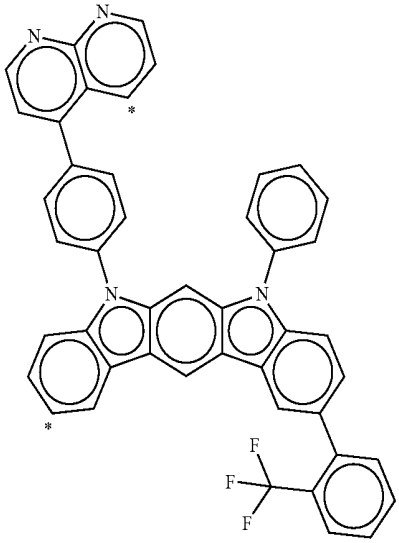


TABLE O-continued

O97



O98



O99

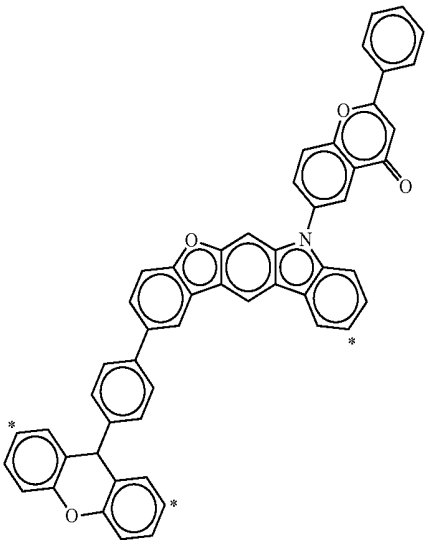
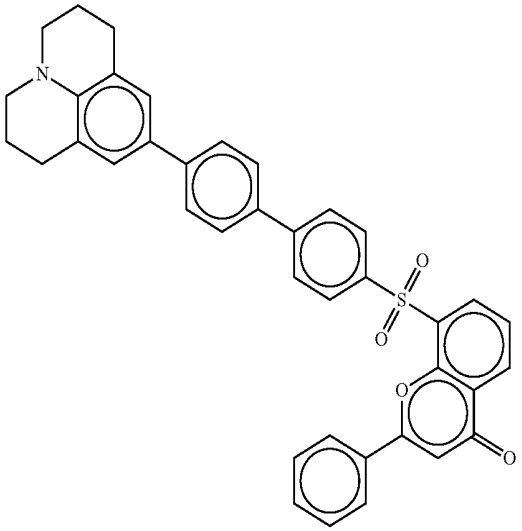


TABLE O-continued

O100



O101

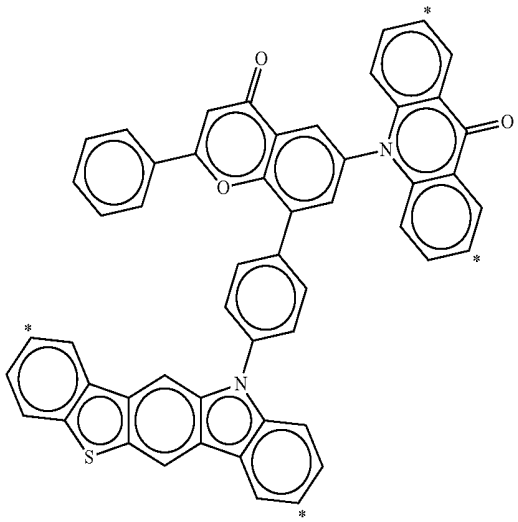
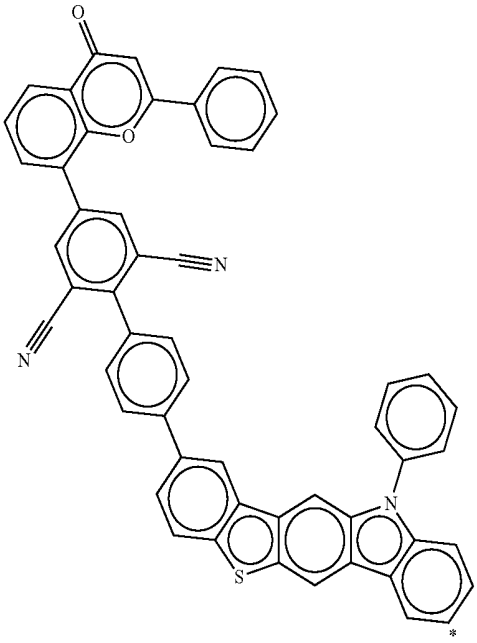


TABLE O-continued

O102



O103

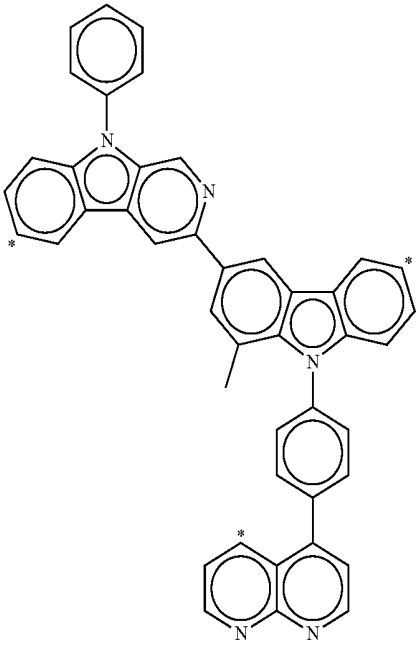
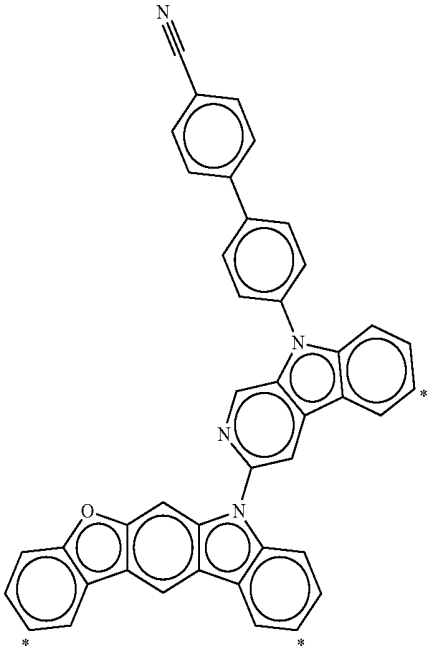


TABLE O-continued

O104



O105

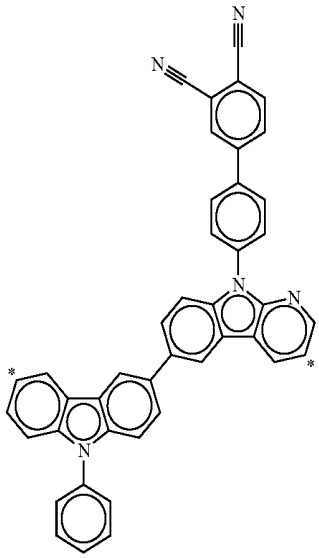
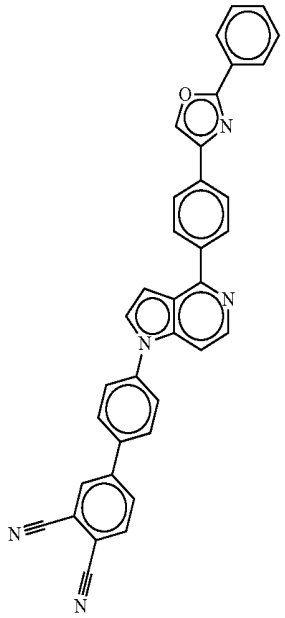


TABLE O-continued

O106



O107

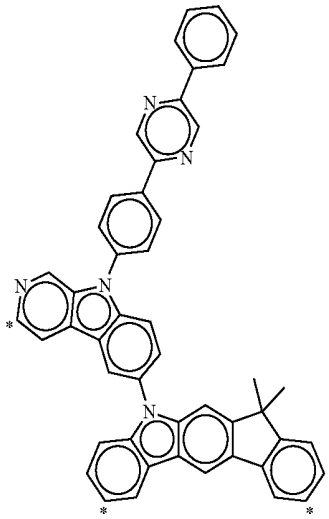


TABLE O-continued

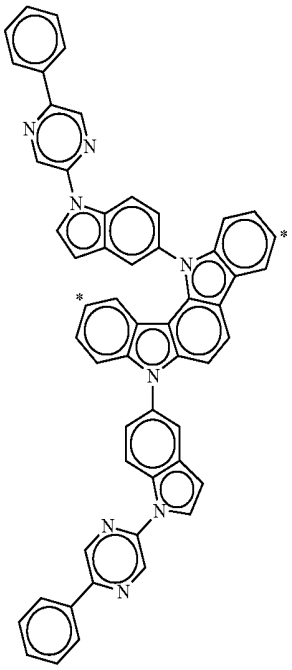
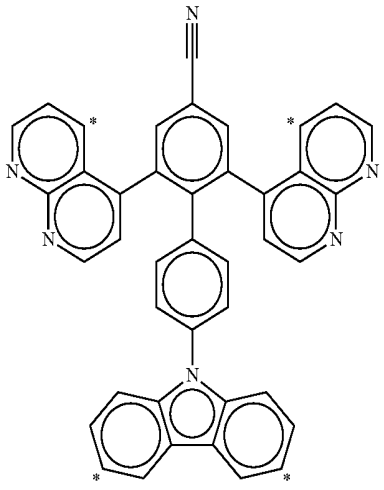
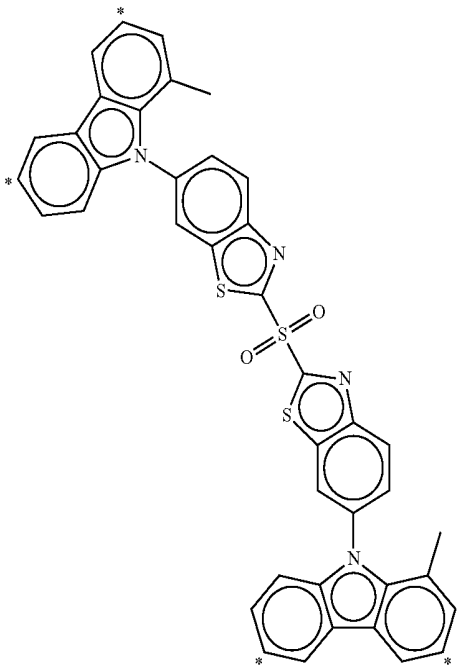
O108	
O109	

TABLE O-continued

O110



O111

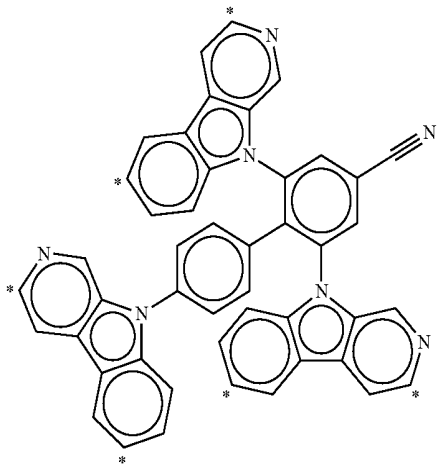
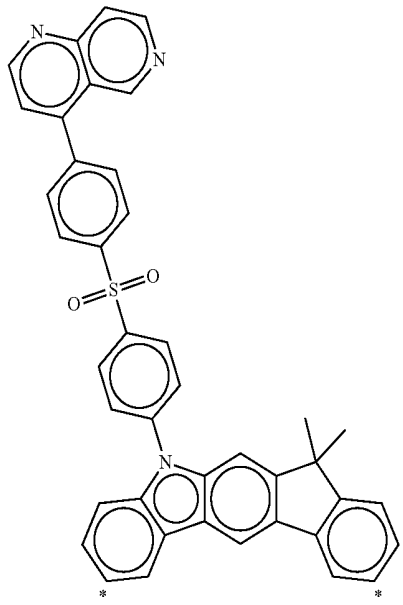


TABLE O-continued

O112



O113

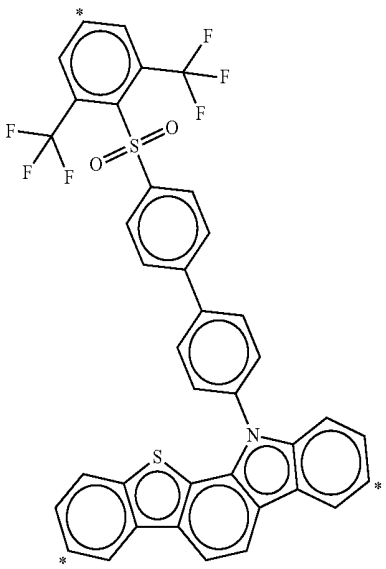
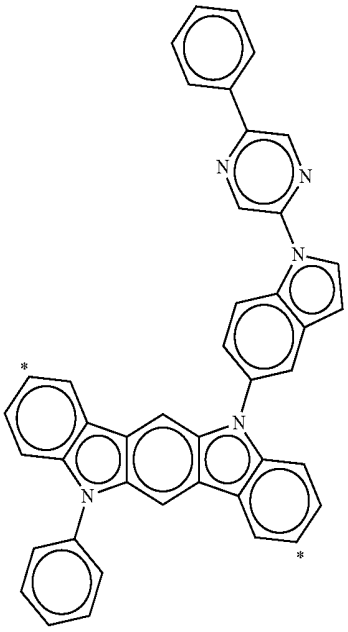


TABLE O-continued

O114



O115

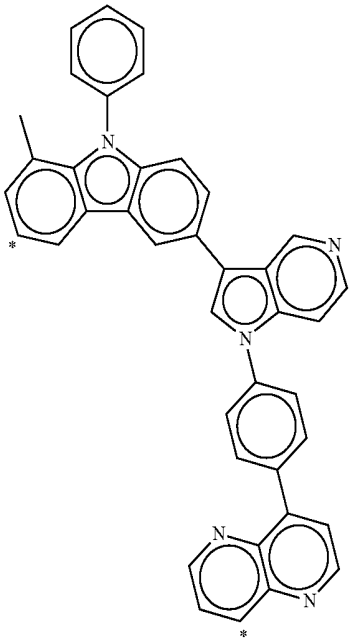
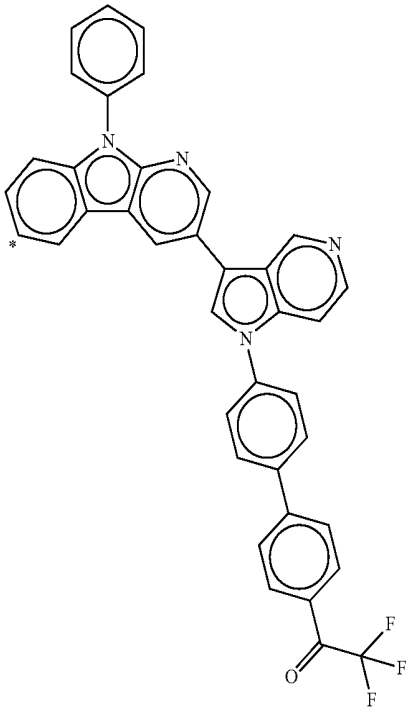


TABLE O-continued

O116



O117

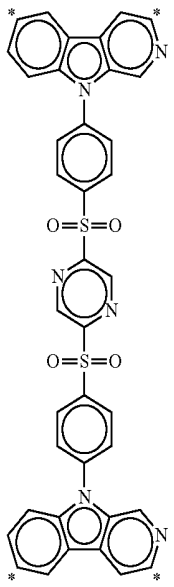
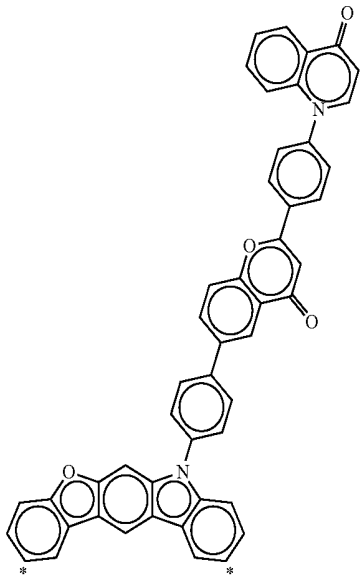
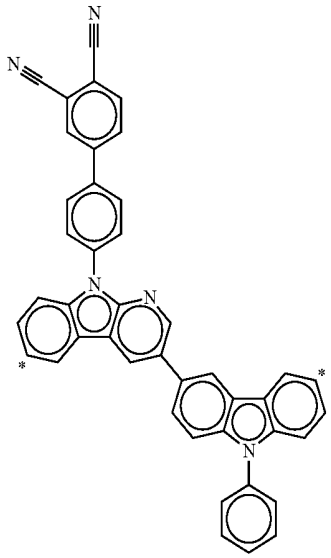


TABLE O-continued

O118



O119



O120

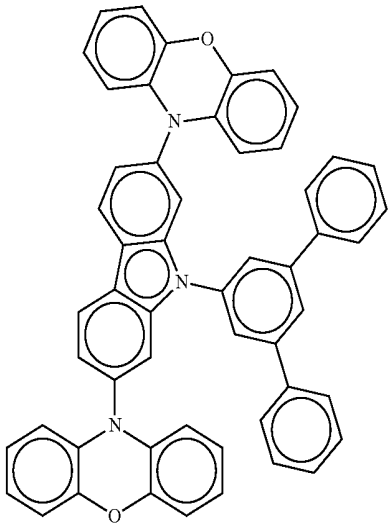
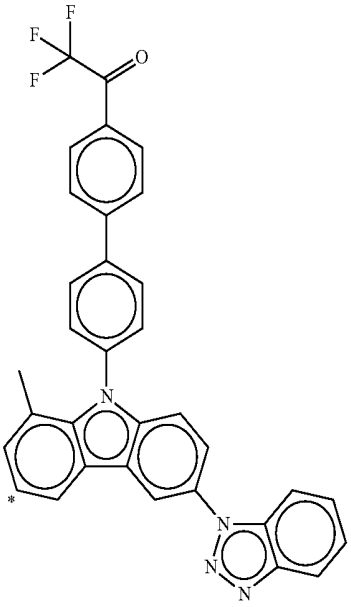


TABLE O-continued

O121



O122

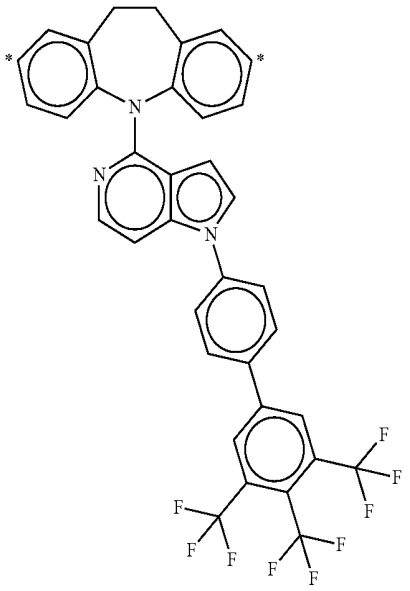
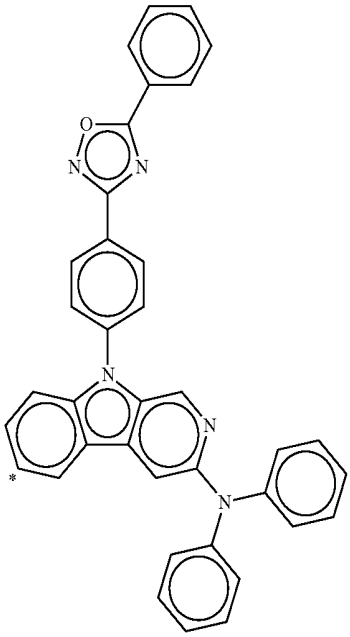


TABLE O-continued

O123	

[0189] In example embodiments of the fourteenth aspect, the present invention is a molecule selected from compounds Q1 to Q12, listed in Table Q. The variables and substitution patterns on the molecule may be selected as described above with respect to the fourteenth aspect. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE Q

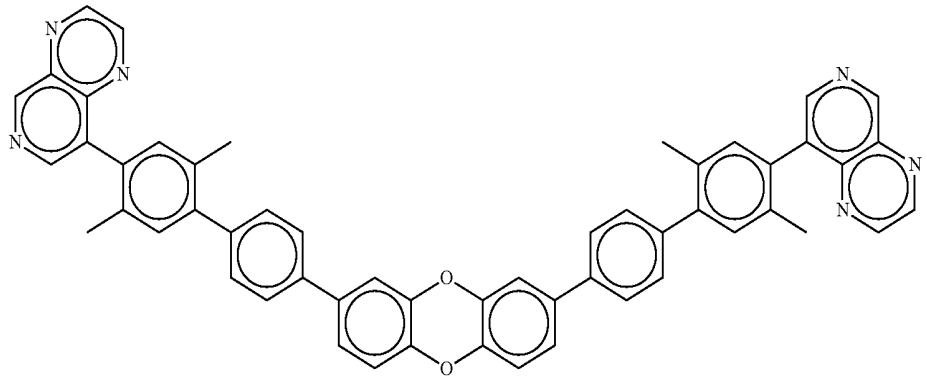
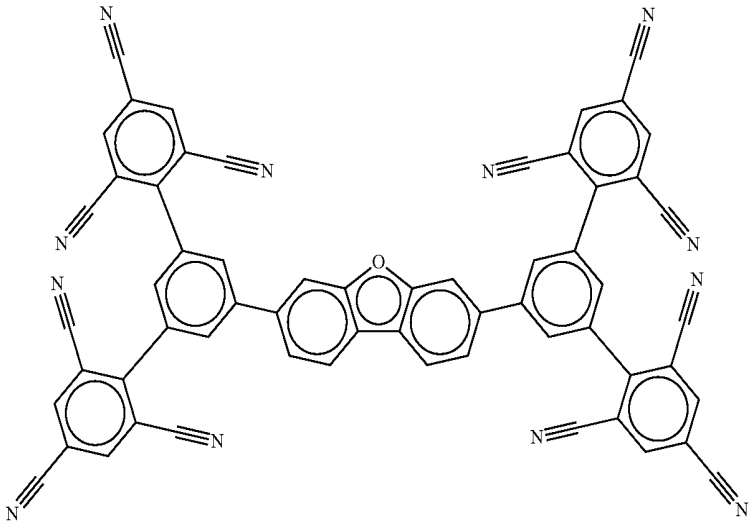
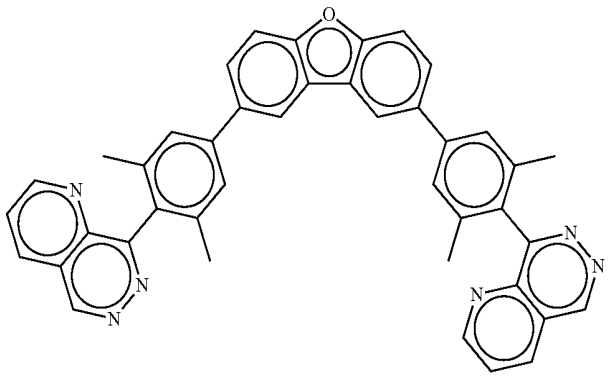
Q1	

TABLE Q-continued

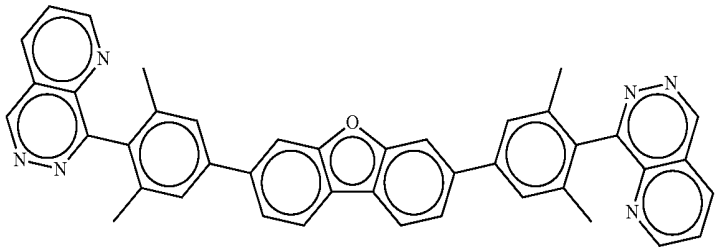
Q2



Q3



Q4



Q5

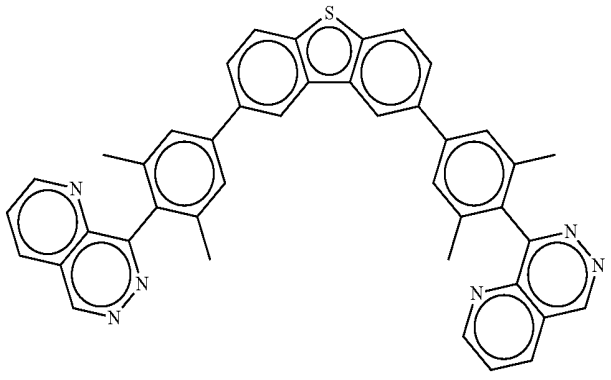
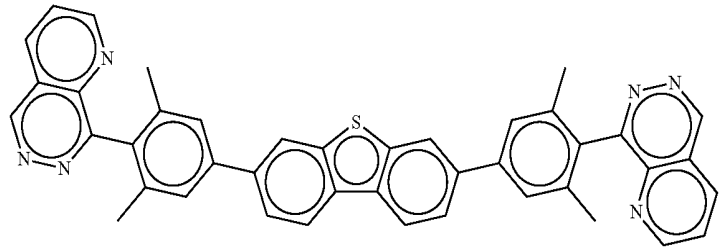
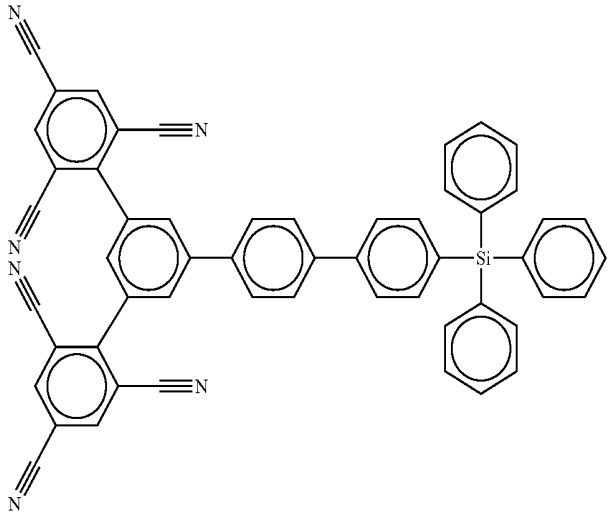


TABLE Q-continued

Q6



Q7



Q8

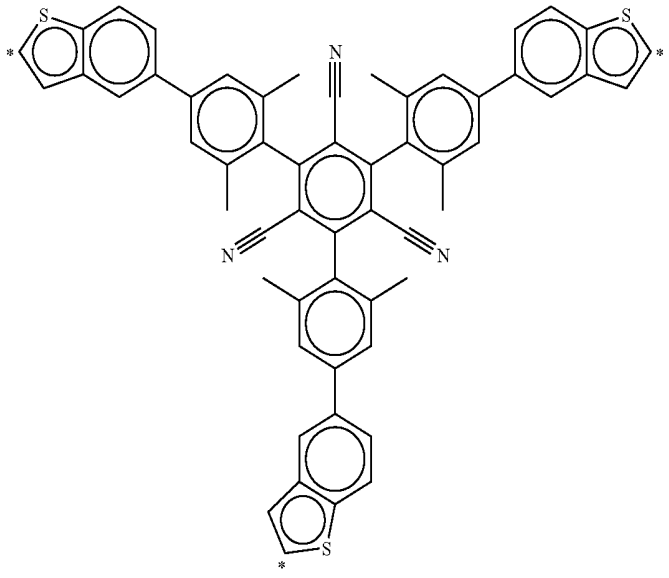
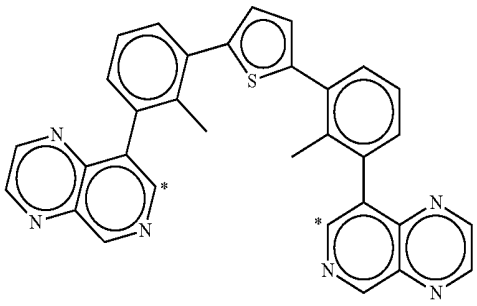
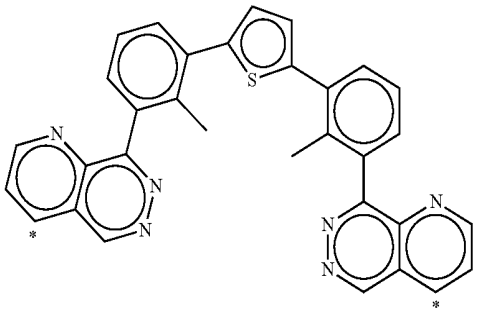


TABLE Q-continued

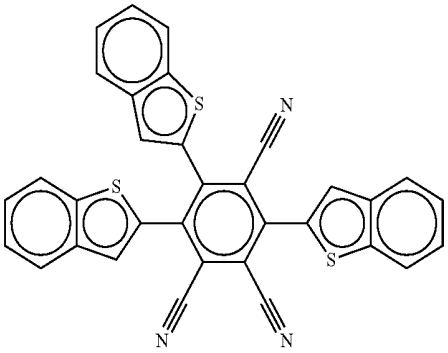
Q9



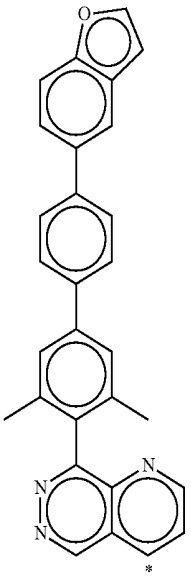
Q10



Q11



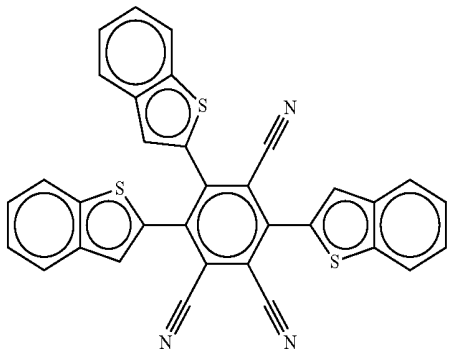
Q12



[0190] In example embodiments of the fourteenth aspect, the present invention is the molecule of Table Q'. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE Q'

Q11



[0191] In example embodiments of the fourteenth aspect, the present invention is any one molecule selected from compounds B1 to B35, listed in Table B. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE B

B1

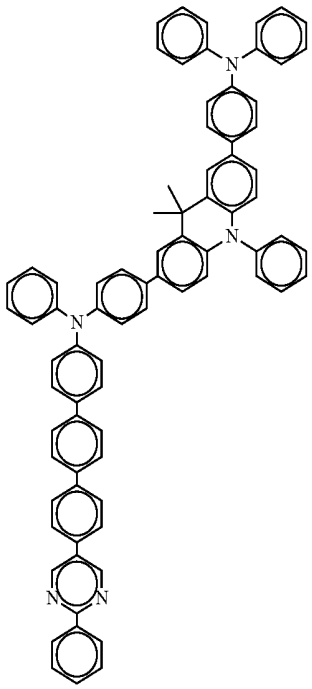
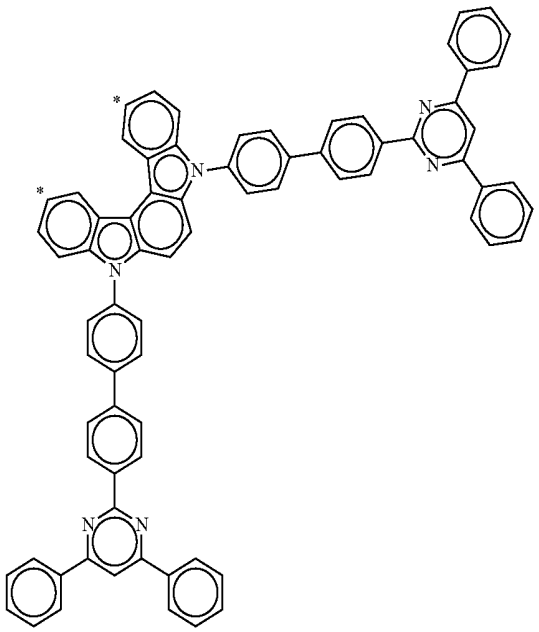


TABLE B-continued

B2



B3

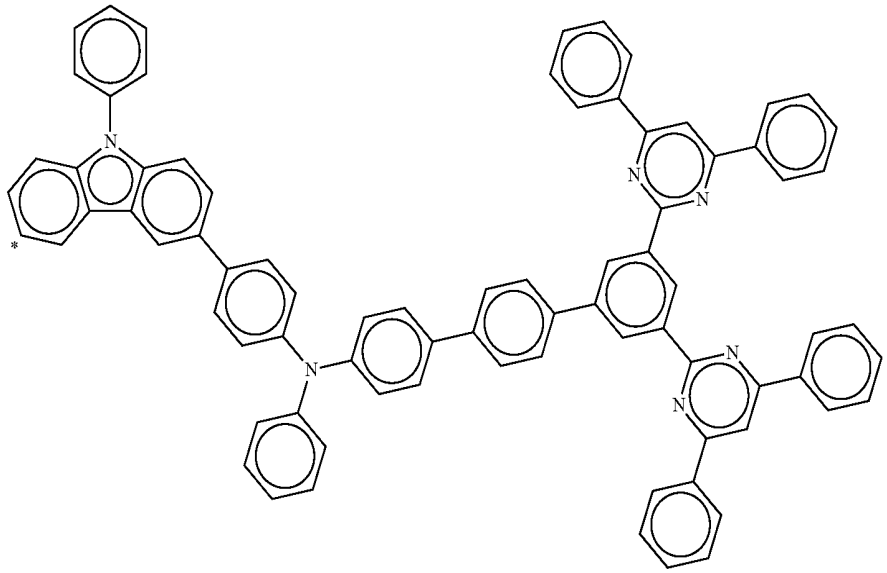
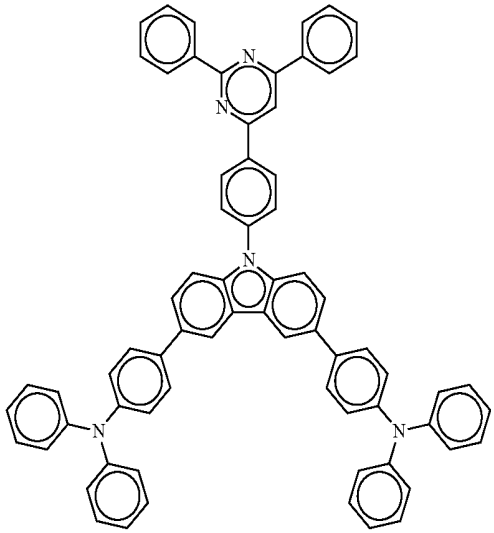


TABLE B-continued

B4



B5

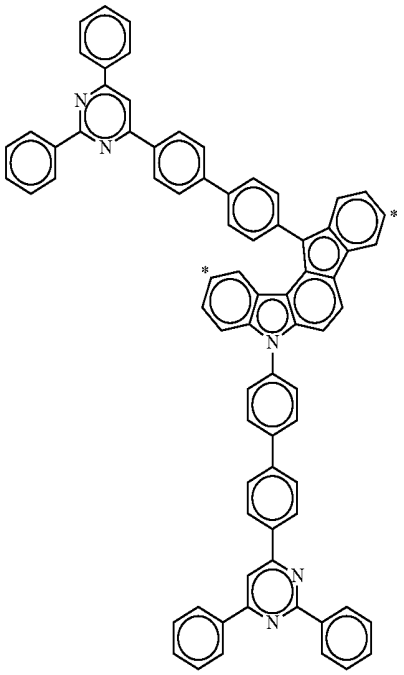
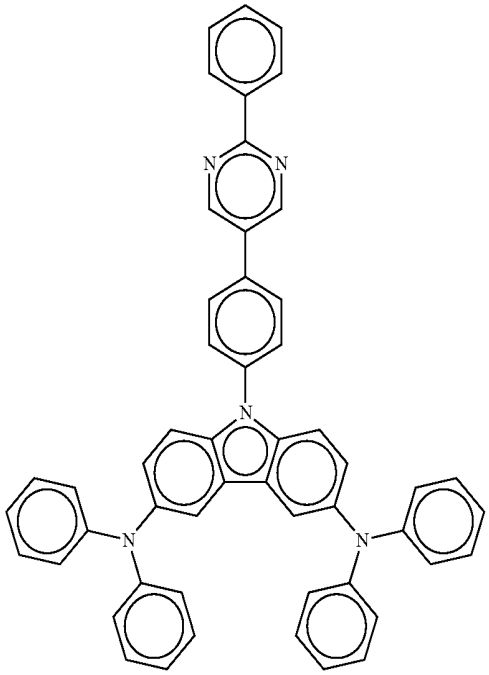


TABLE B-continued

B6



B7

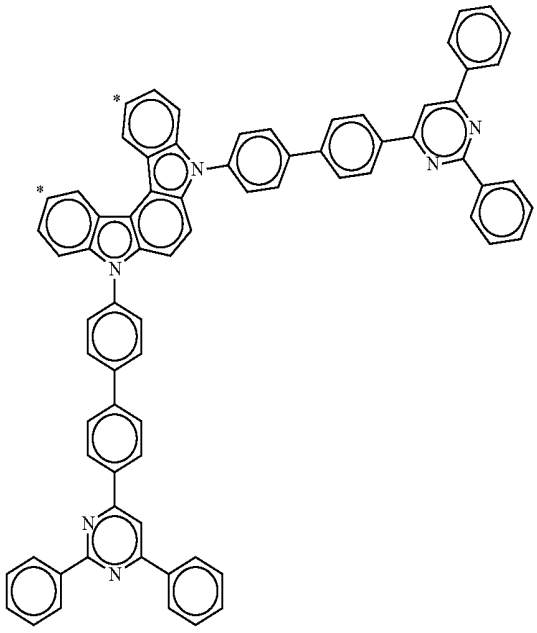
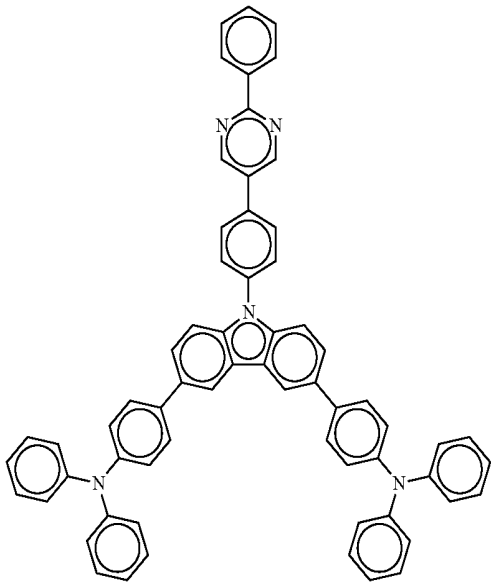
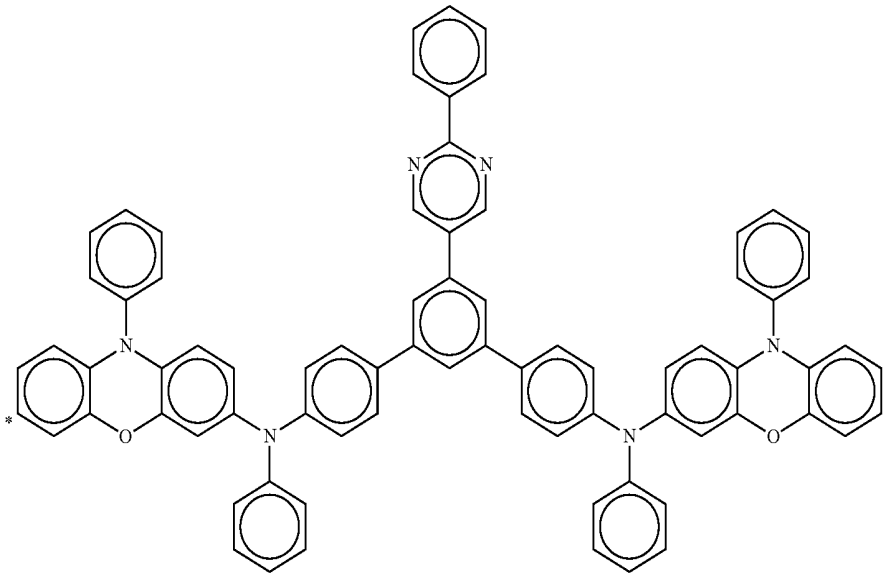


TABLE B-continued

B8



B9



B10

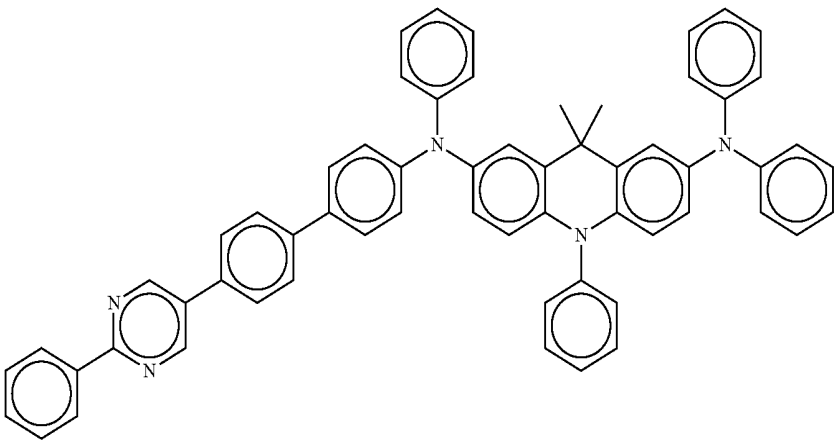
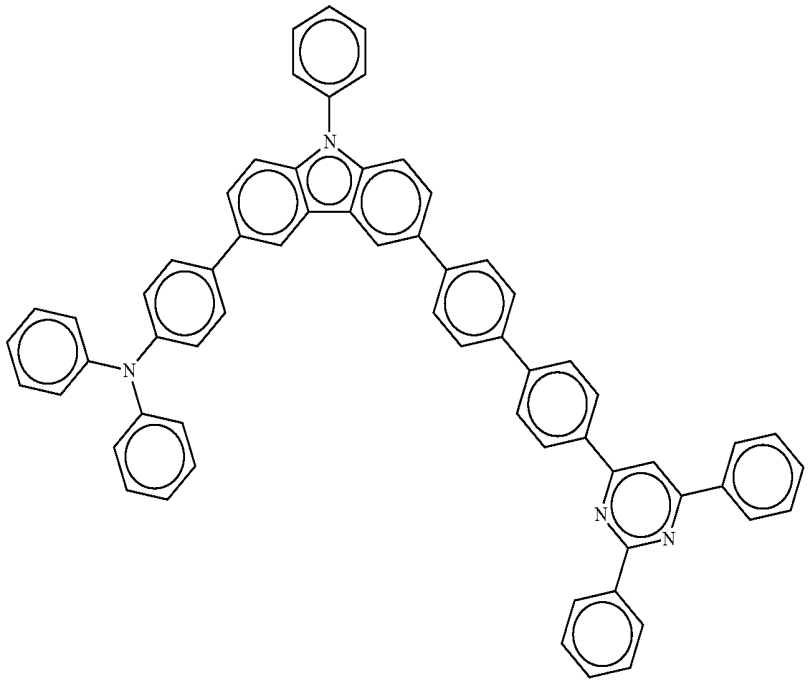


TABLE B-continued

B11



B12

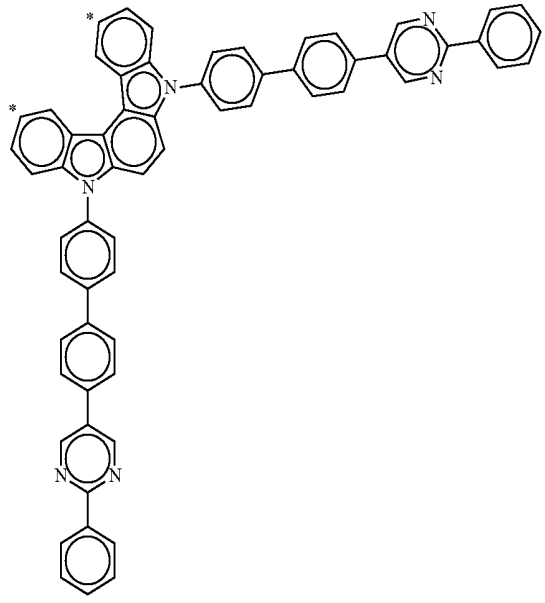
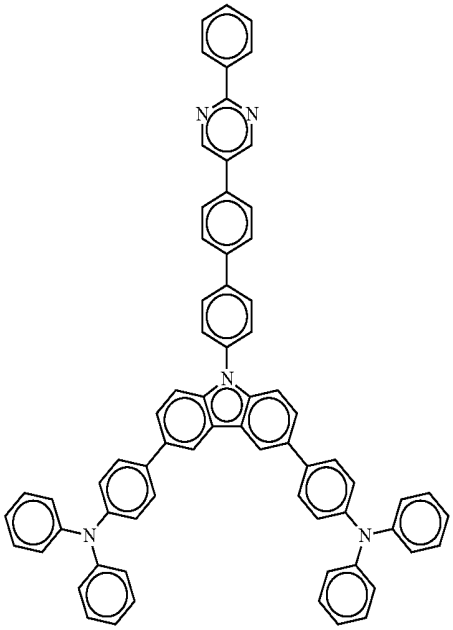


TABLE B-continued

B13



B14

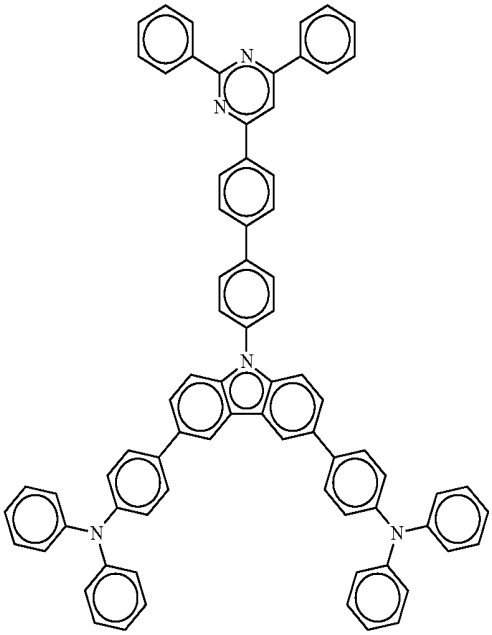
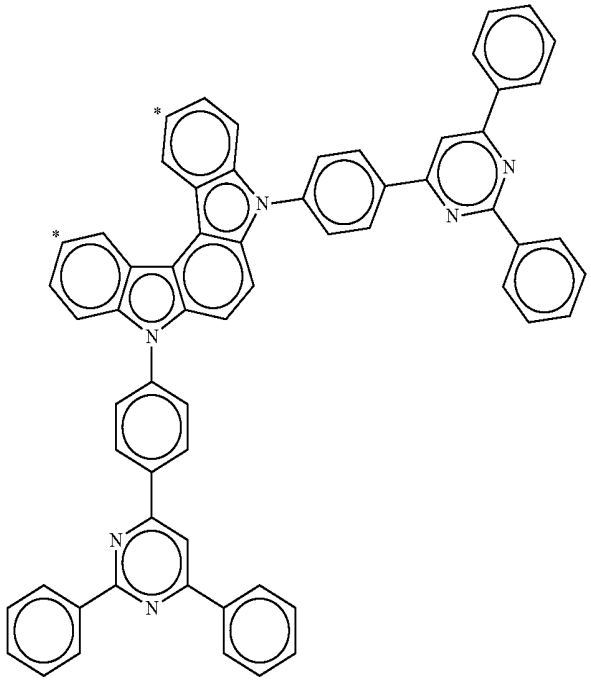


TABLE B-continued

B15



B16

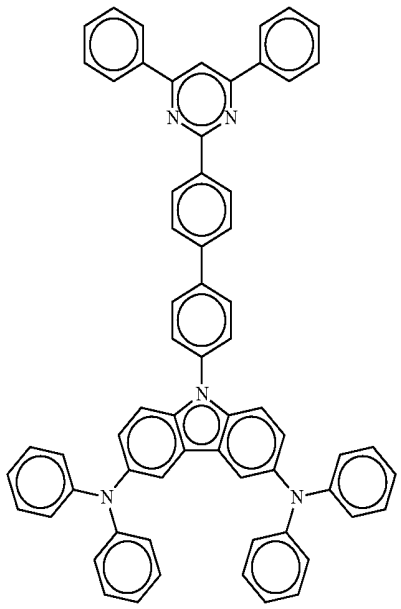
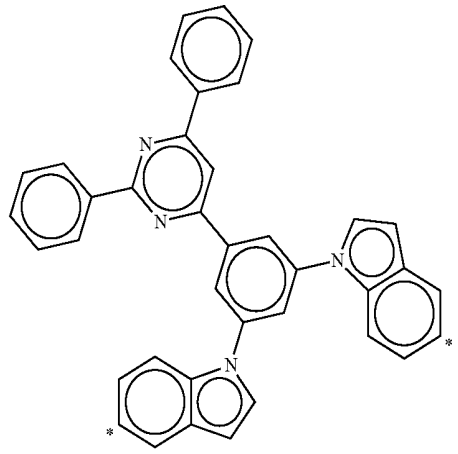
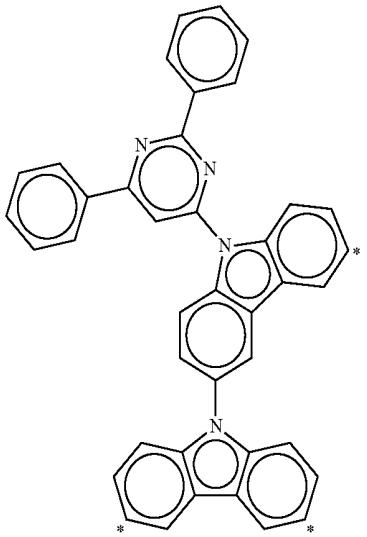


TABLE B-continued

B17



B18



B19

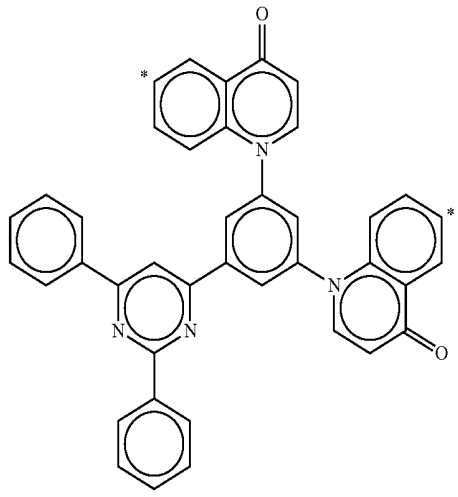
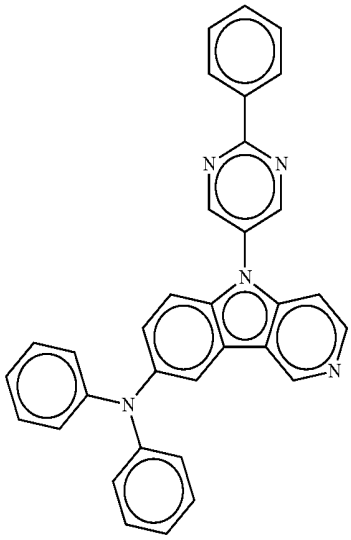
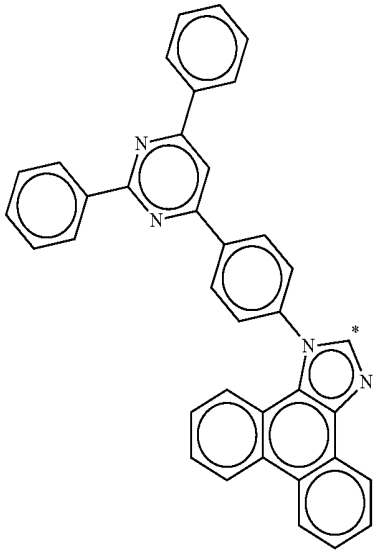


TABLE B-continued

B20



B21



B22

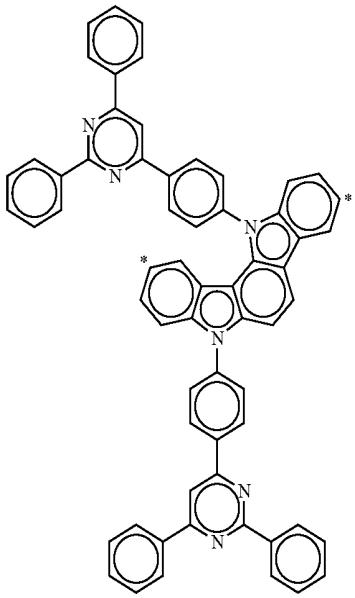
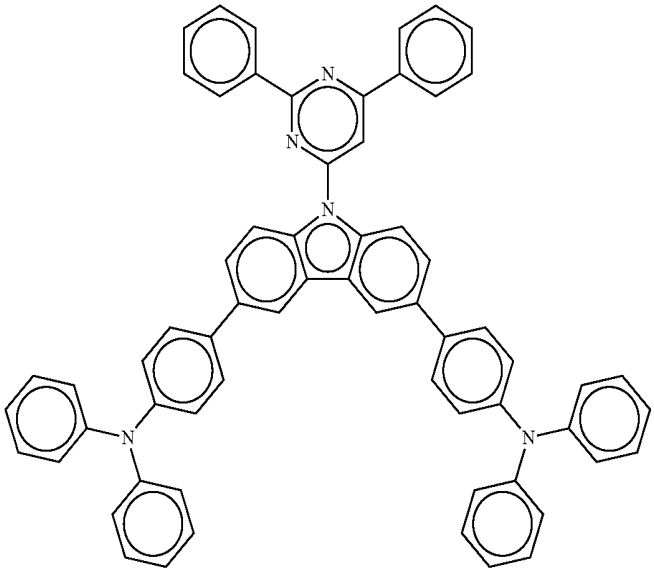
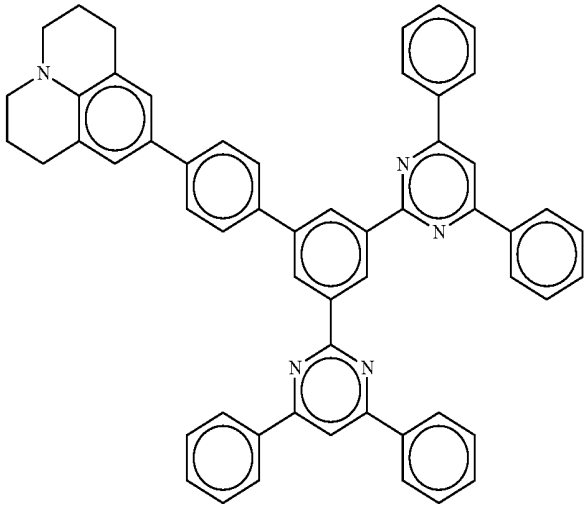


TABLE B-continued

B23



B24



B25

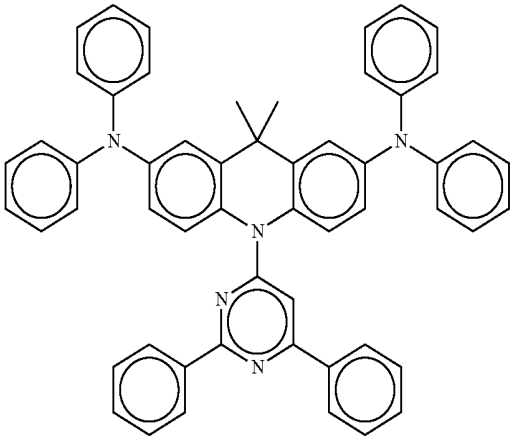
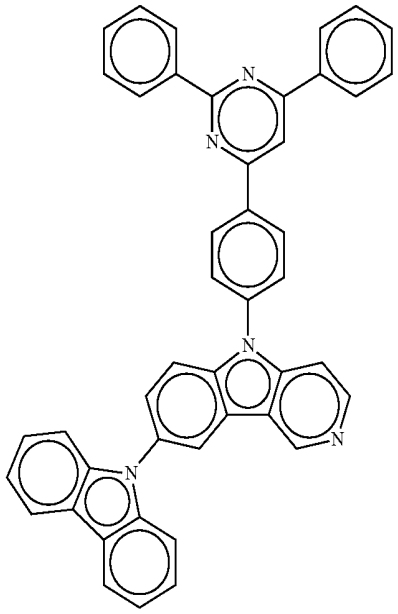


TABLE B-continued

B26



B27

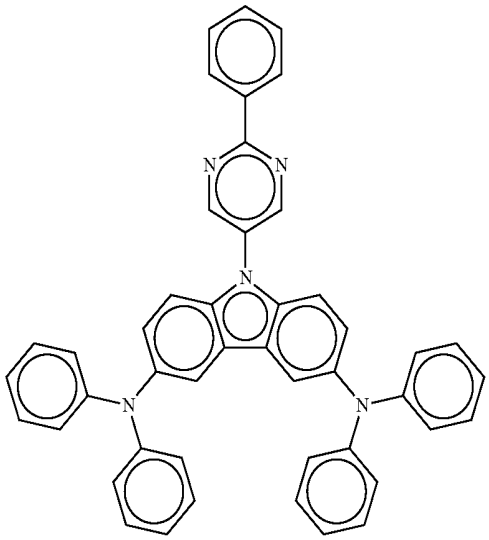
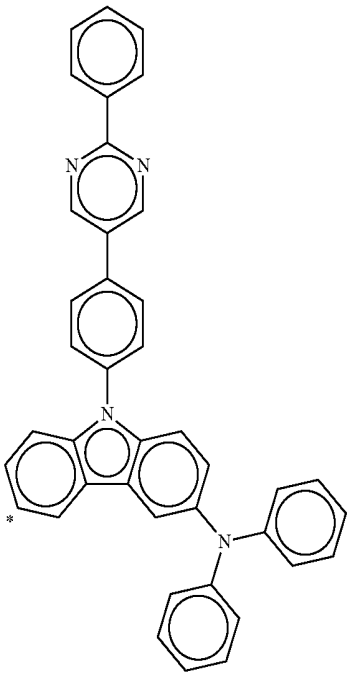


TABLE B-continued

B28



B29

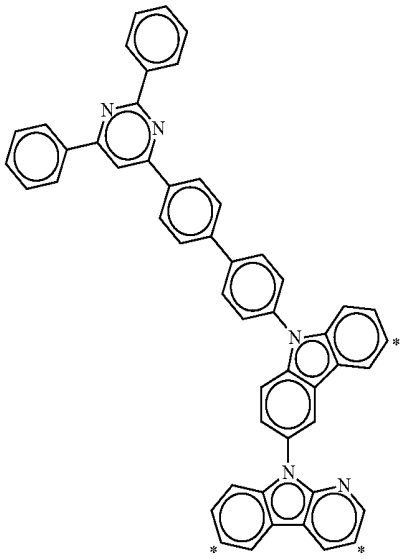
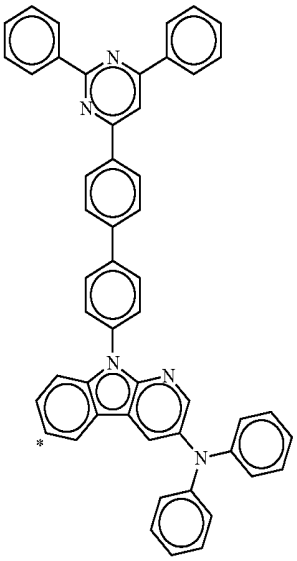


TABLE B-continued

B30



B31

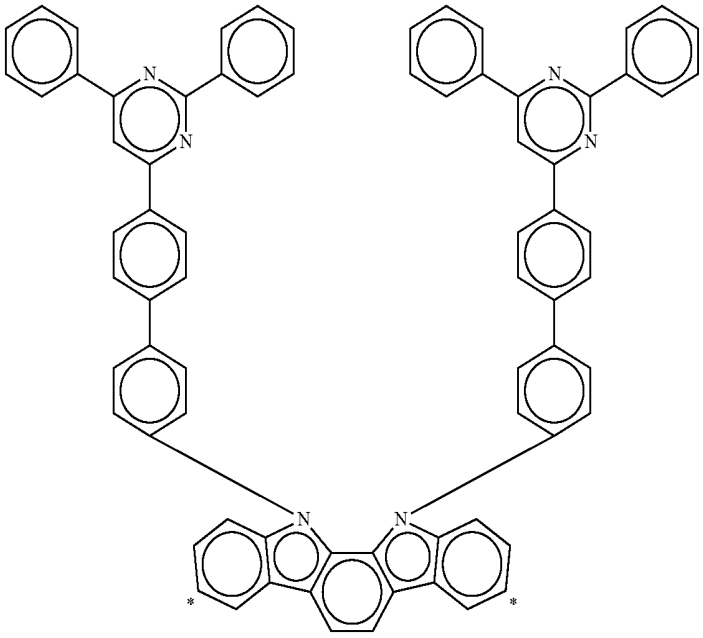
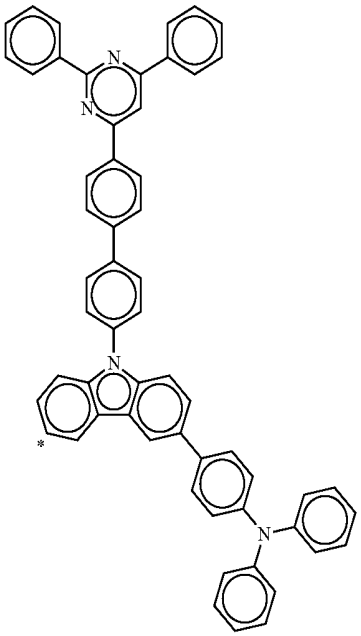
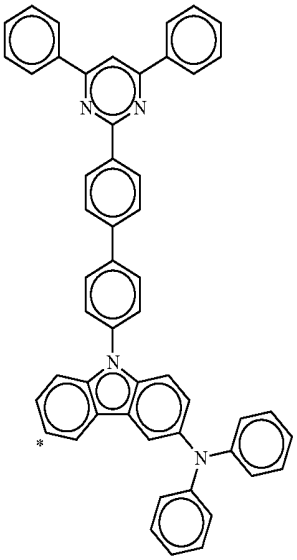


TABLE B-continued

B32



B33



B34

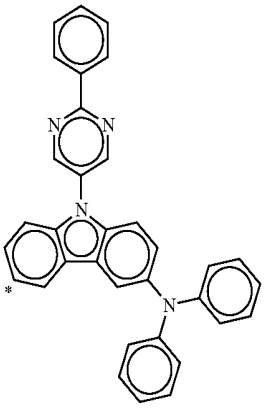
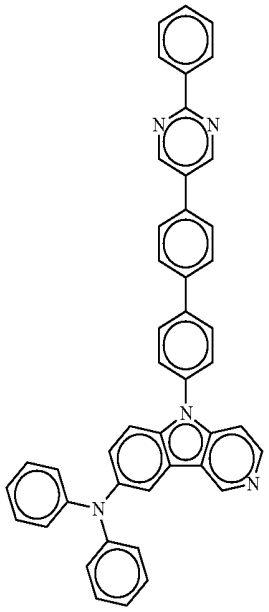


TABLE B-continued

B35	

[0192] In example embodiments of the fourteenth aspect, the present invention is a molecule selected from compounds R1 to R108, listed in Table R. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE R

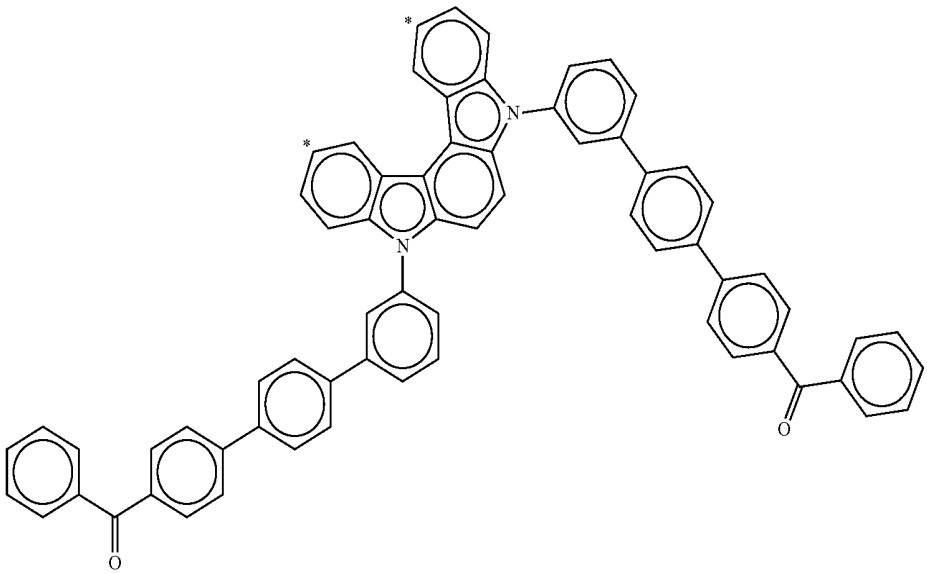
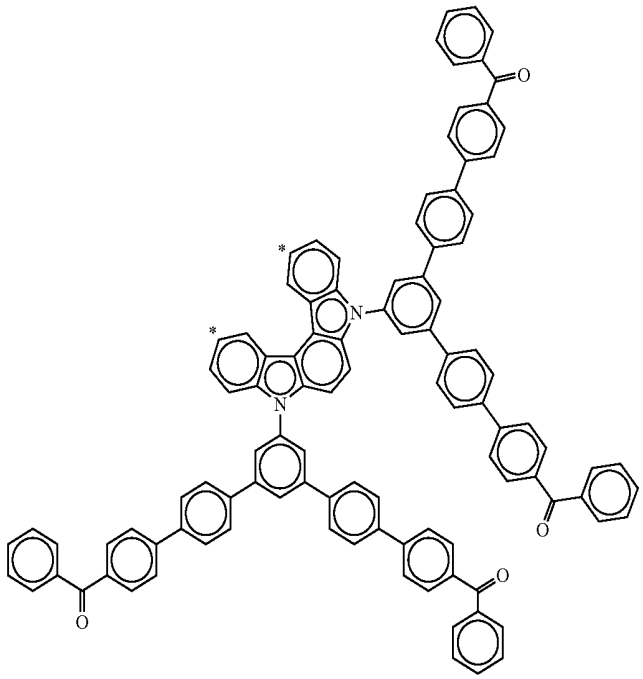
R1	

TABLE R-continued

R2



R3

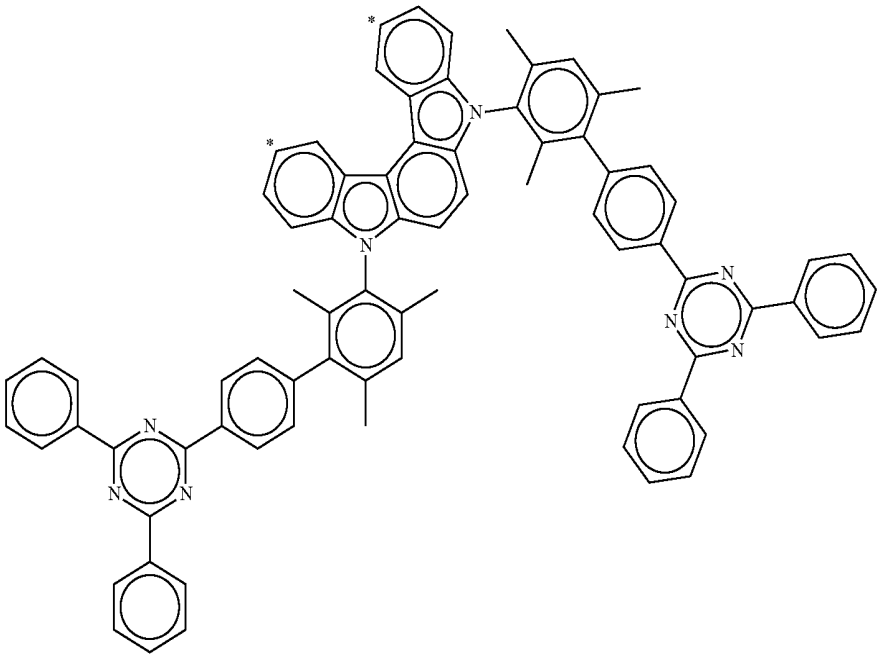
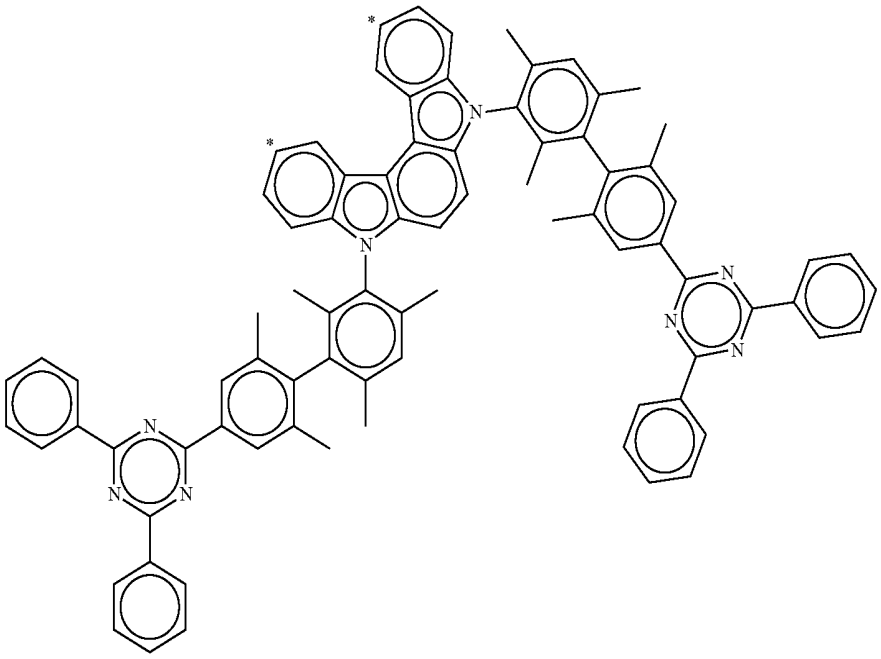


TABLE R-continued

R4



R5

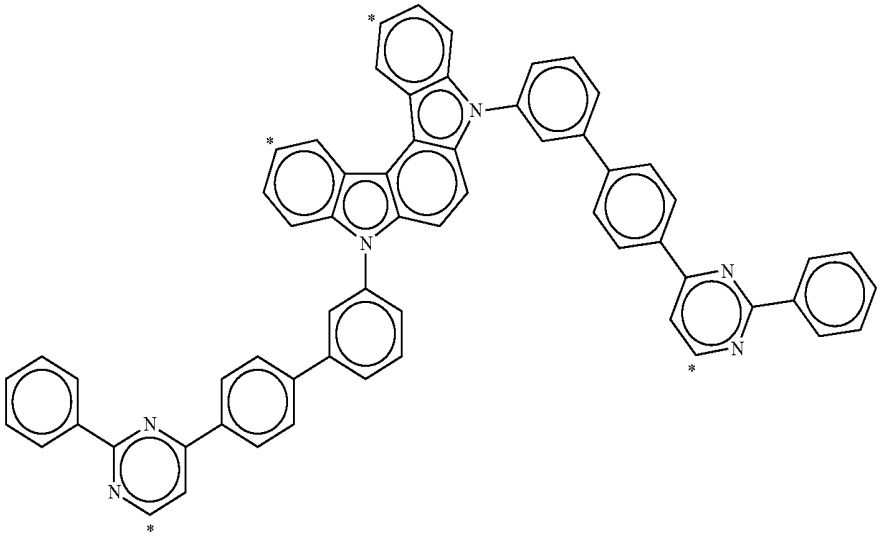
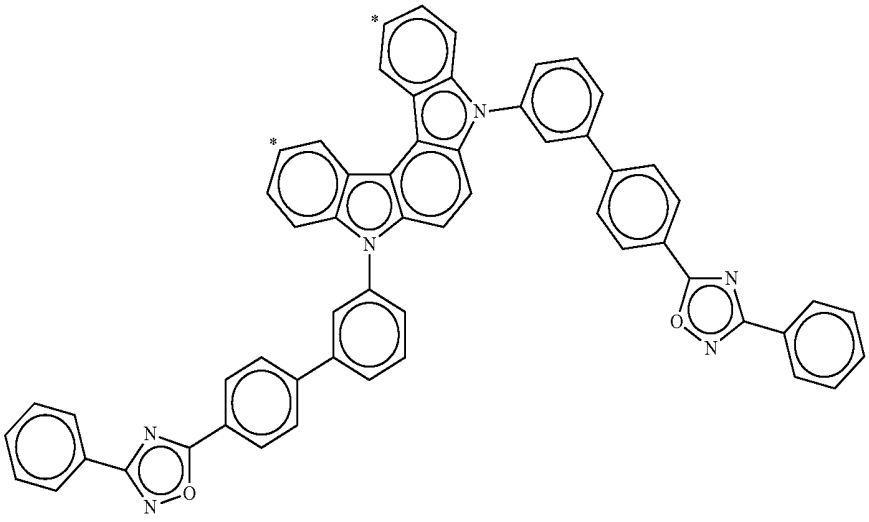


TABLE R-continued

R6



R7

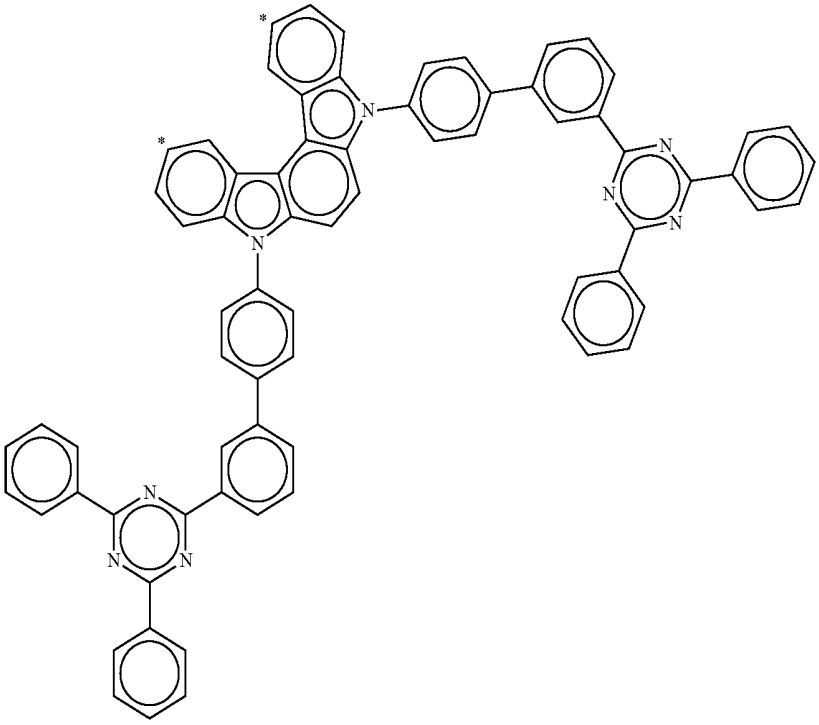
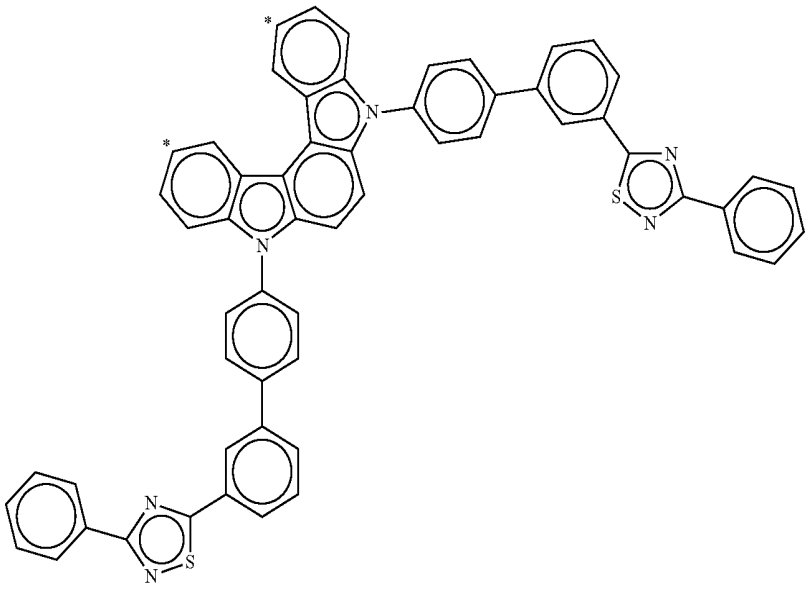


TABLE R-continued

R8



R9

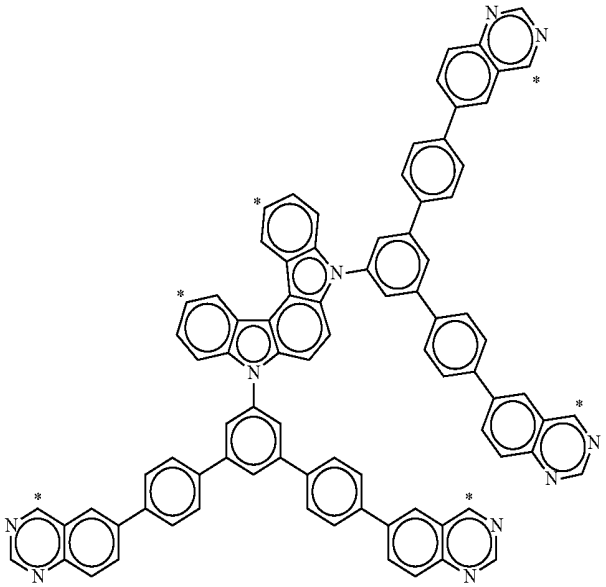
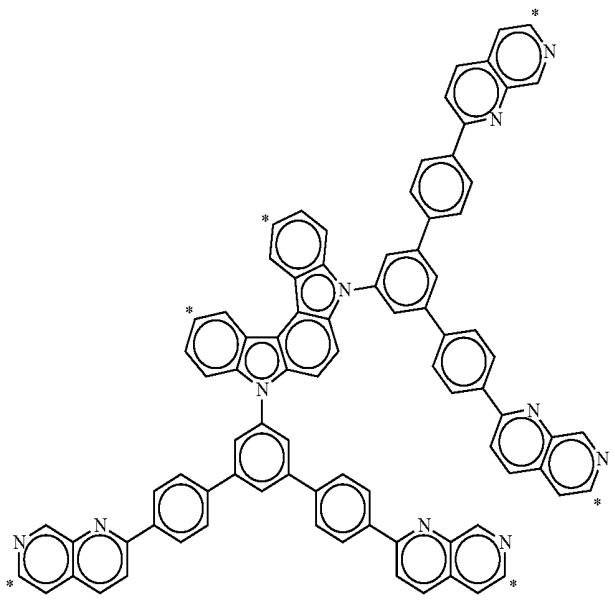


TABLE R-continued

R10



R11

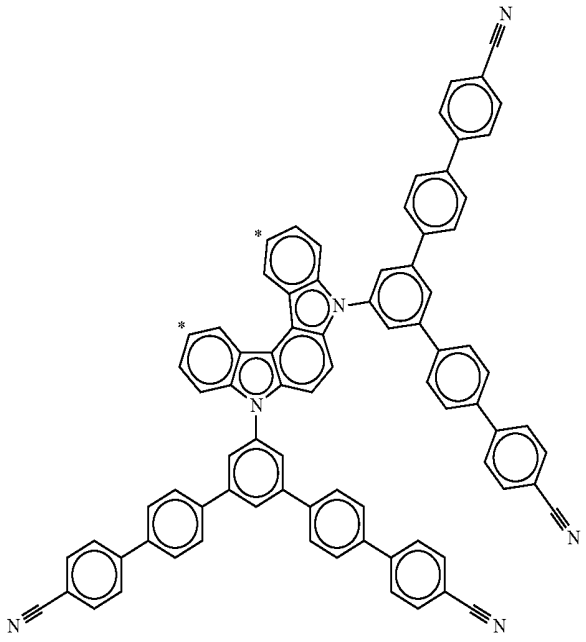
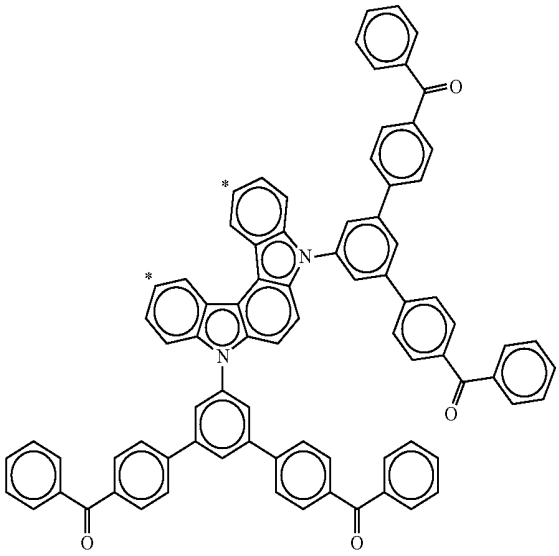
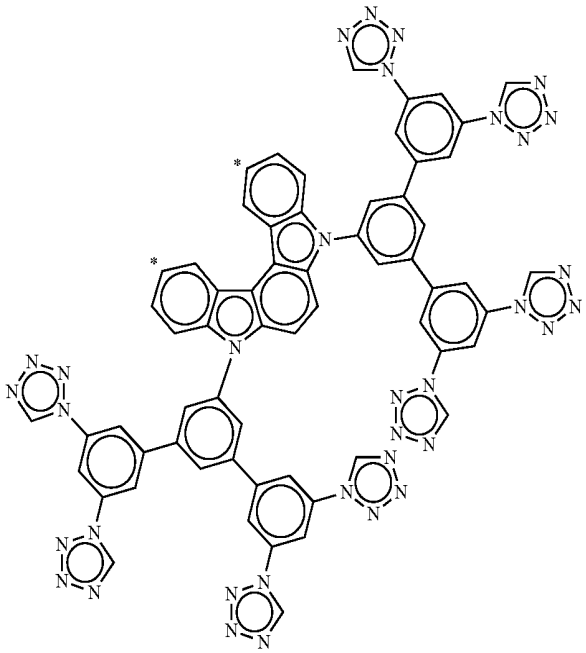


TABLE R-continued

R12



R13



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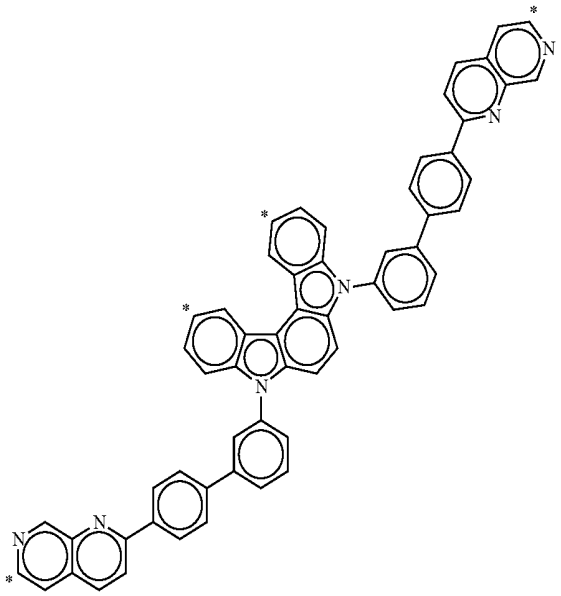
R14



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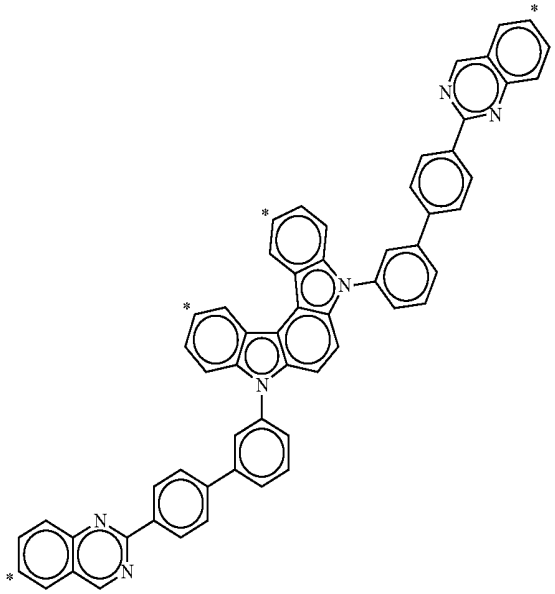

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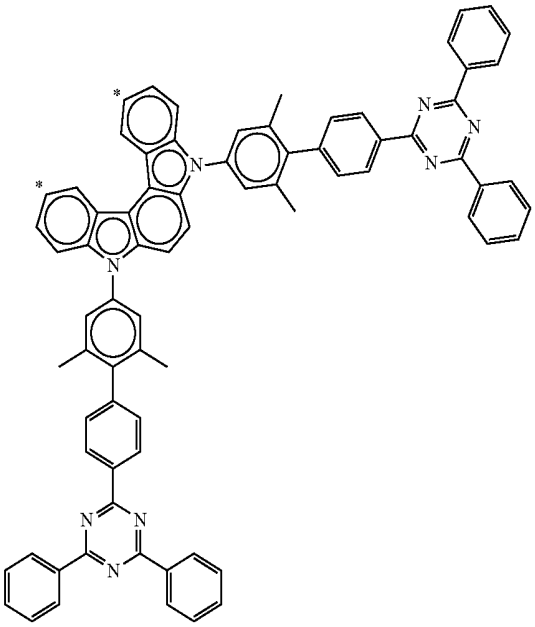
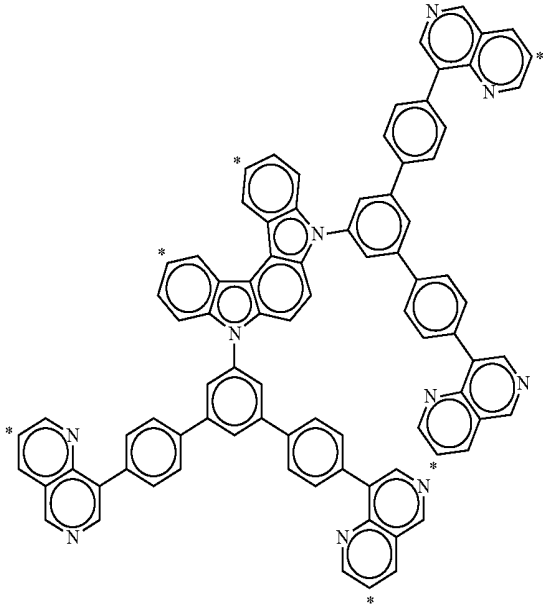


R17



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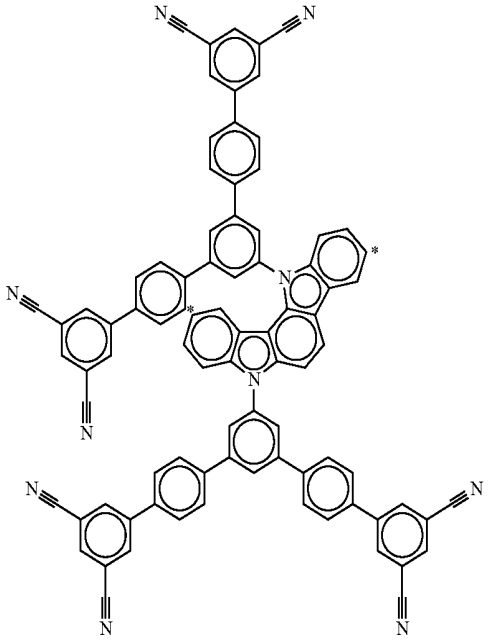
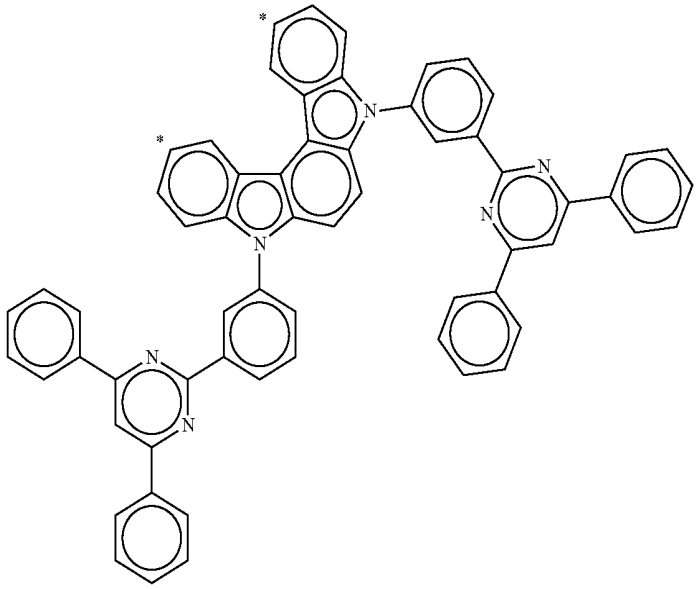
R18



R19



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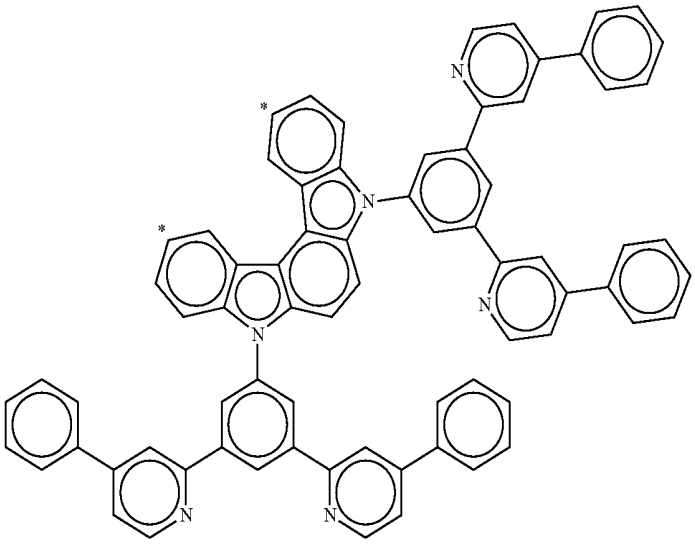

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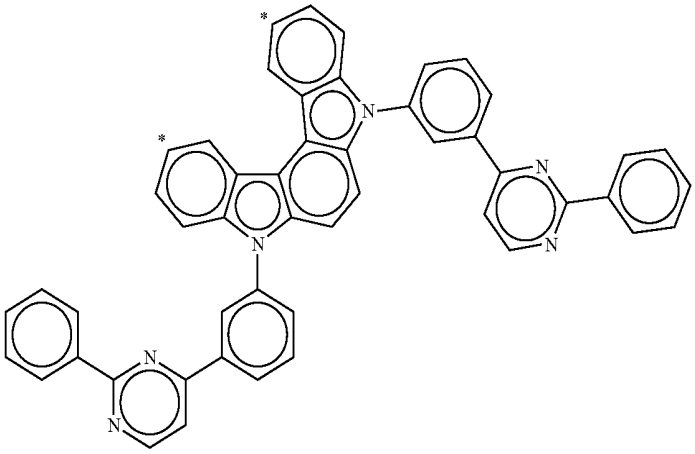

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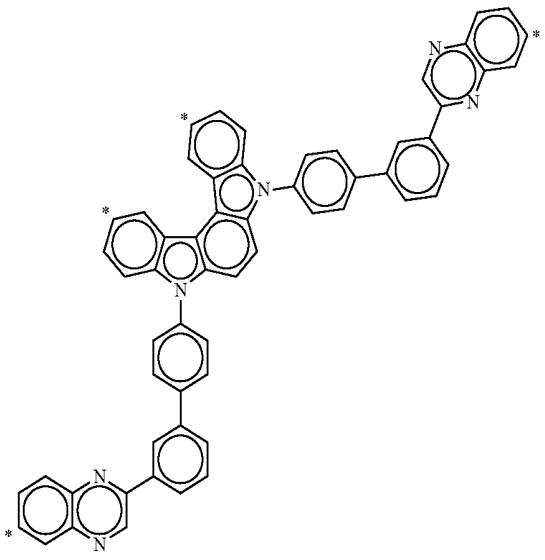

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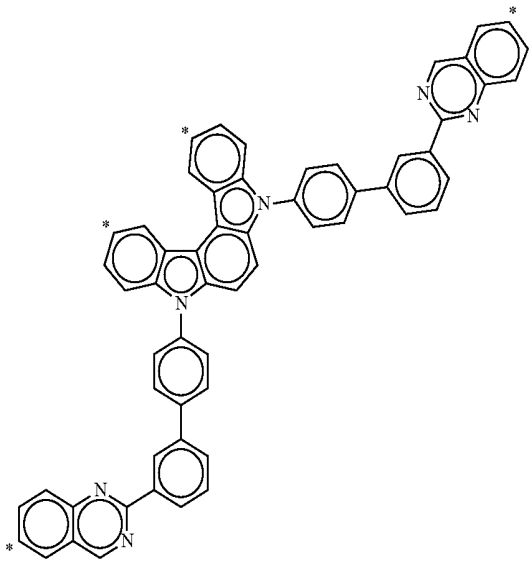
R23



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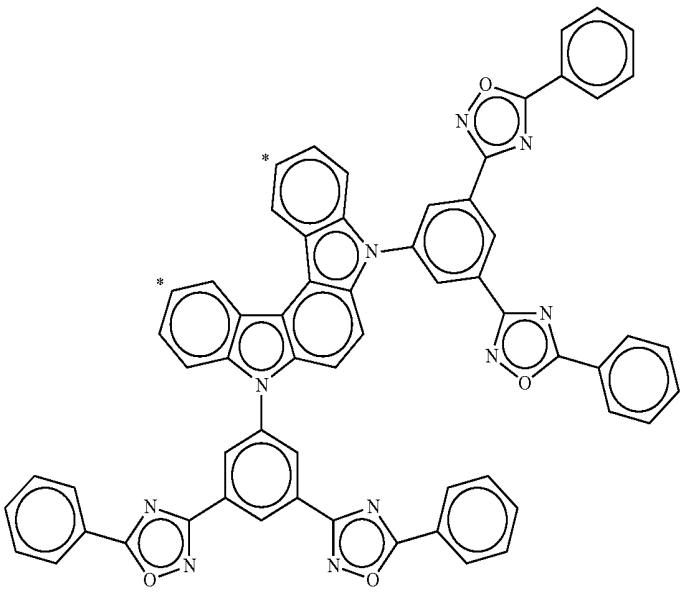

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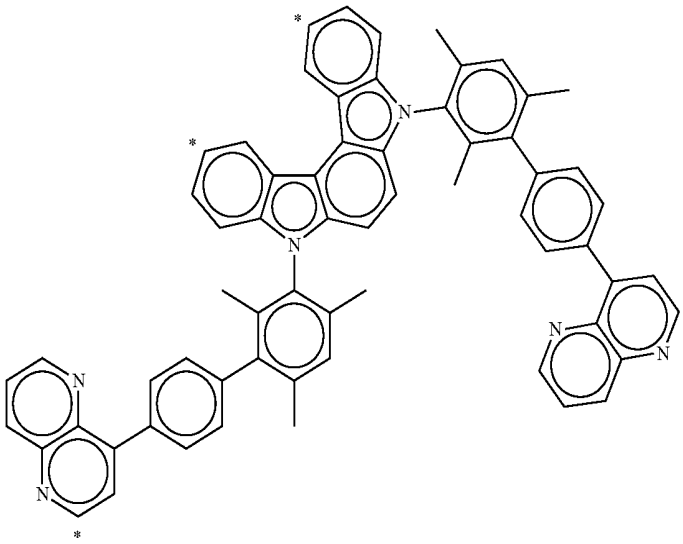

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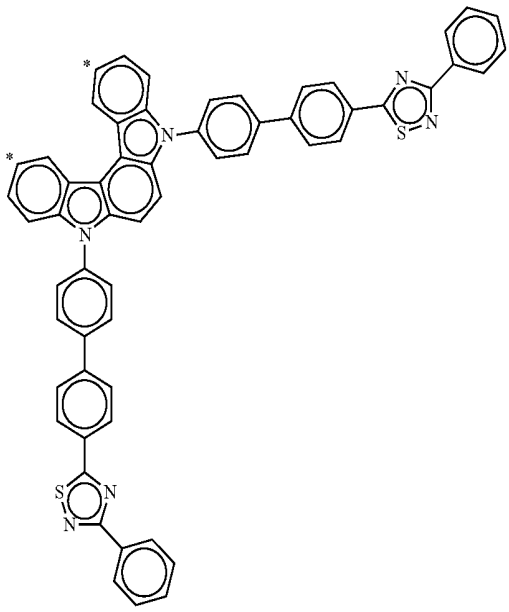

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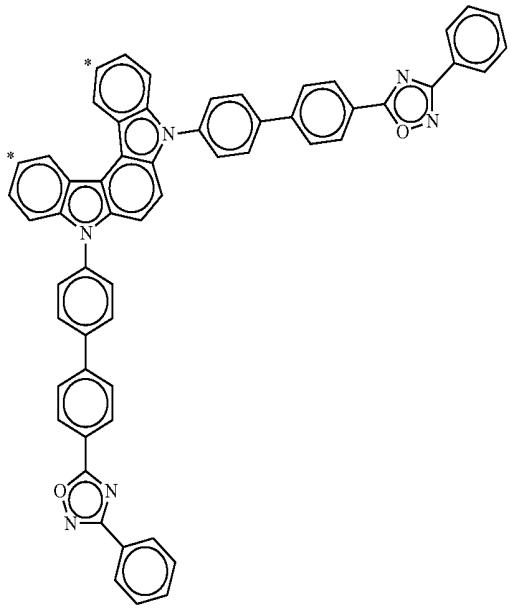
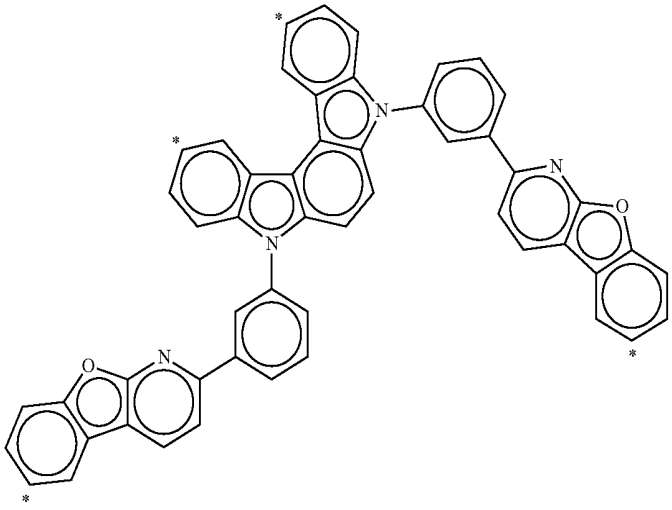
R27



R28



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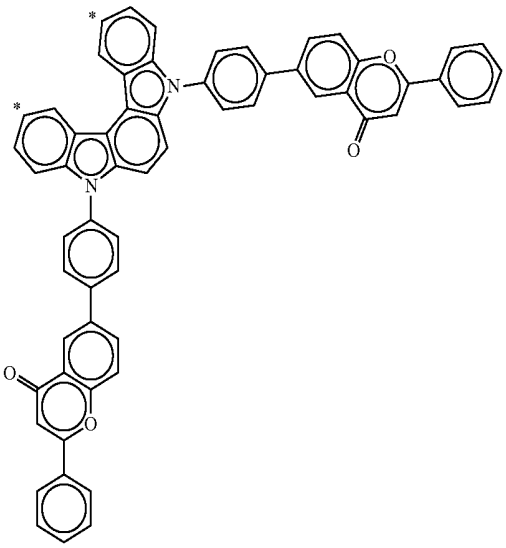

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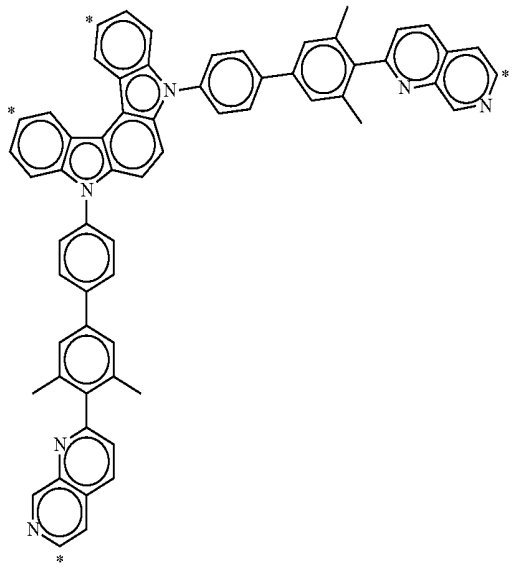
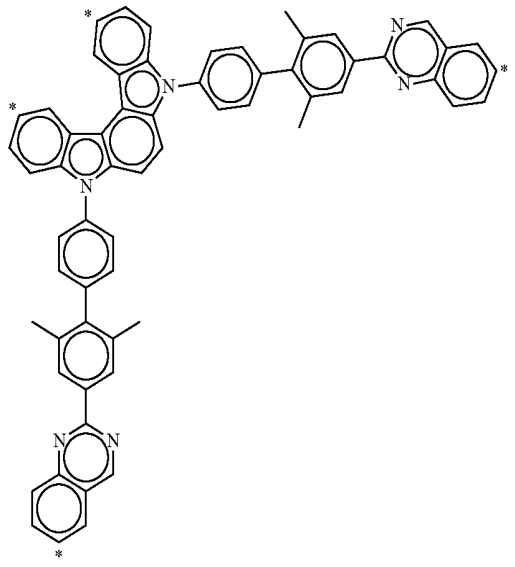
R30



R31



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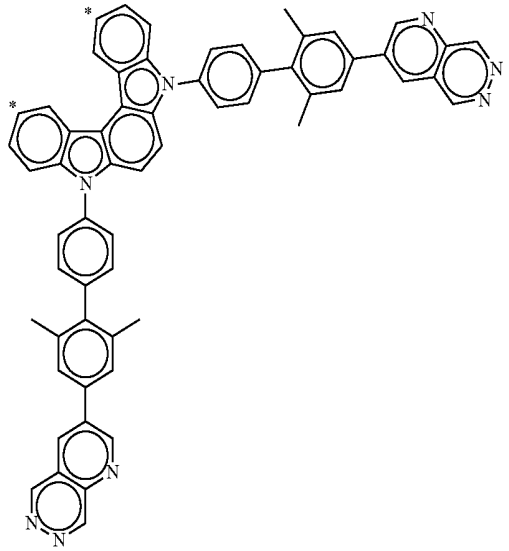
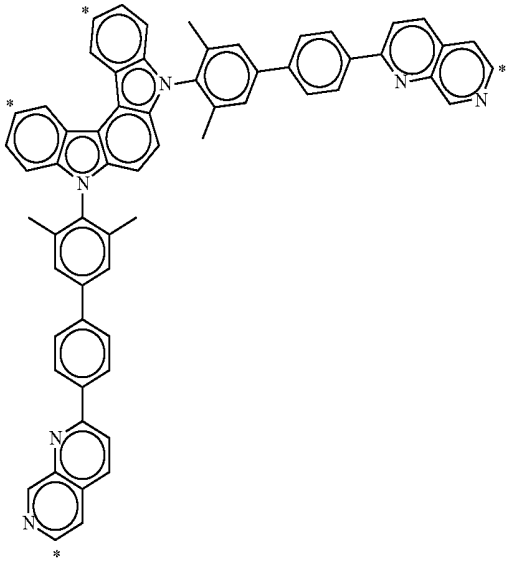
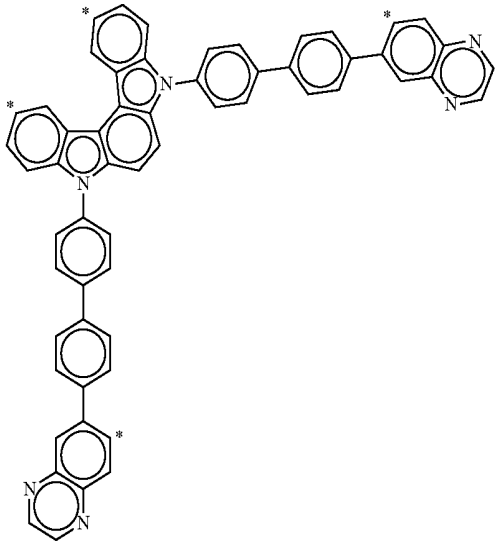
R32



R33



R34



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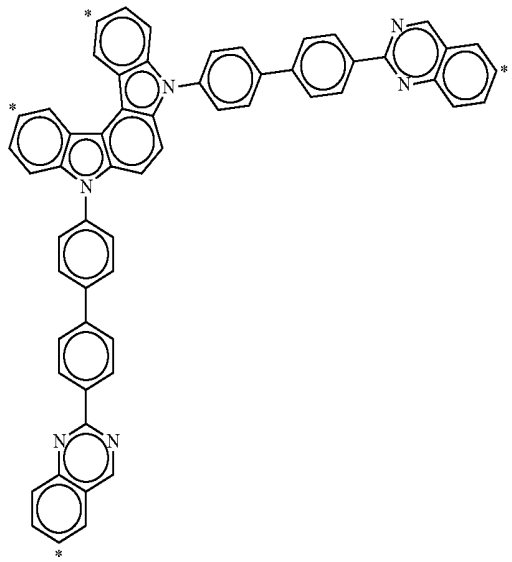
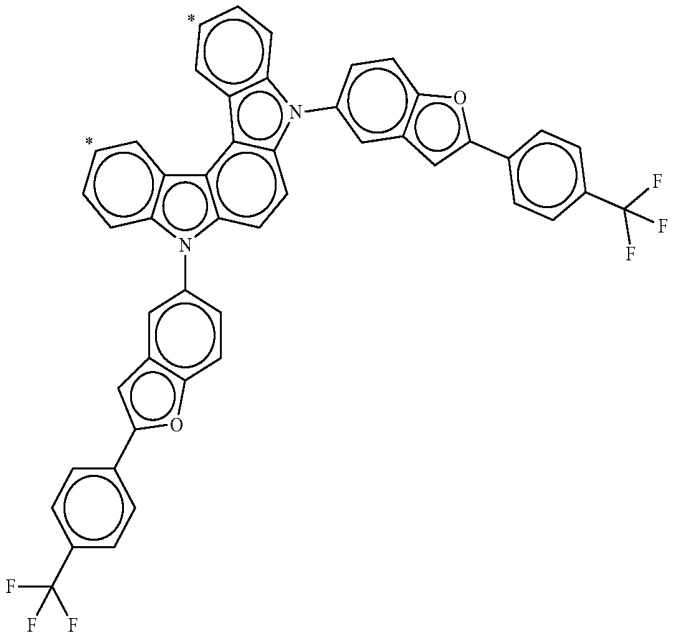
R35



R36



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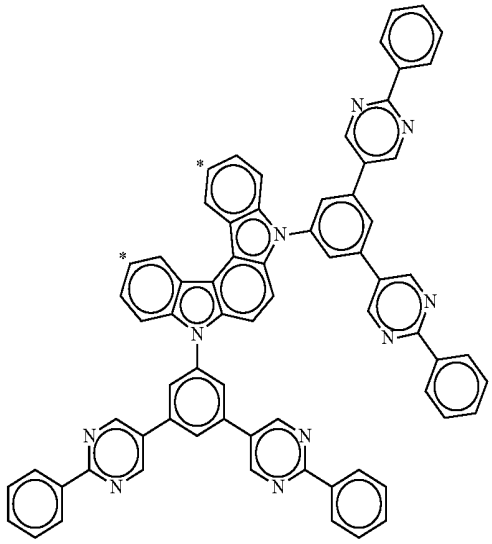
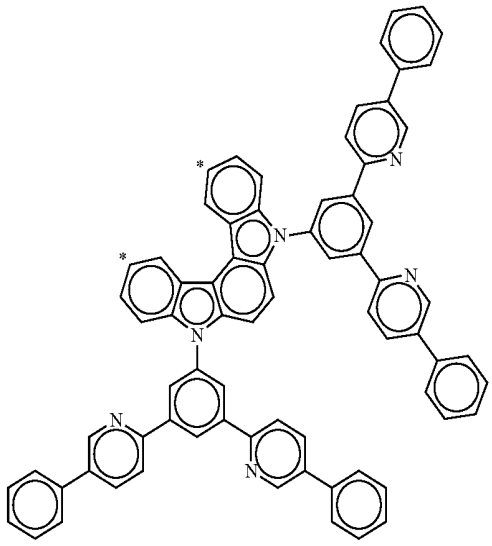
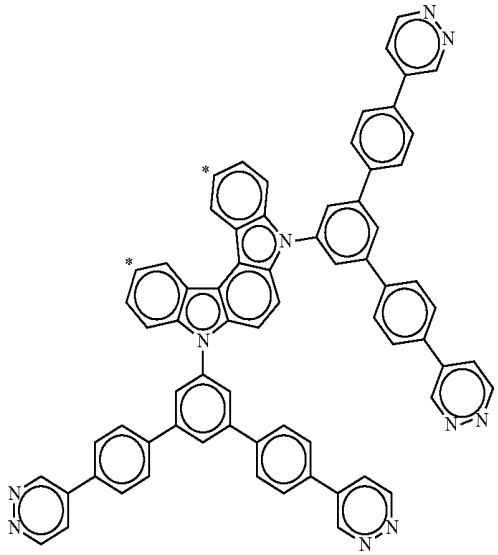
R37



R38



R39



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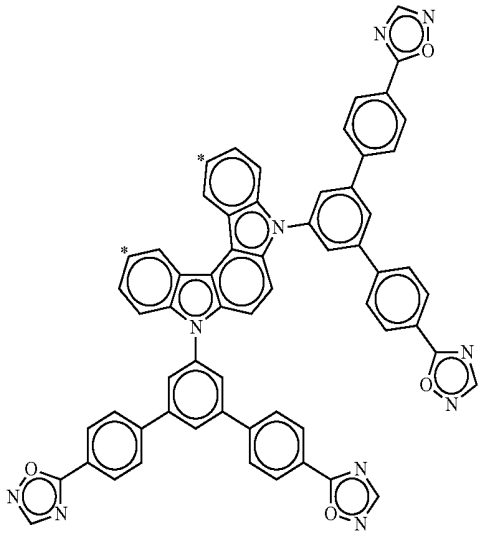
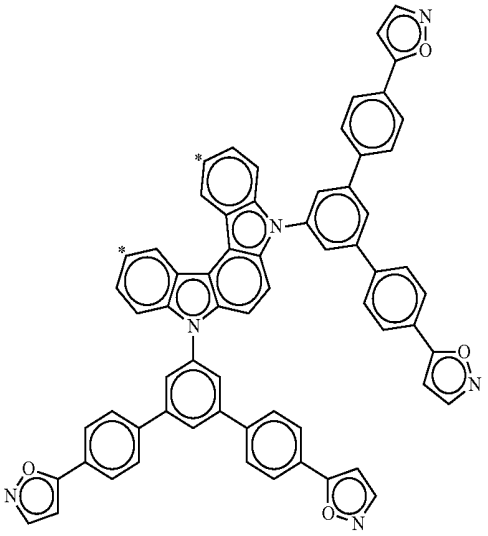
R40



R41



R42

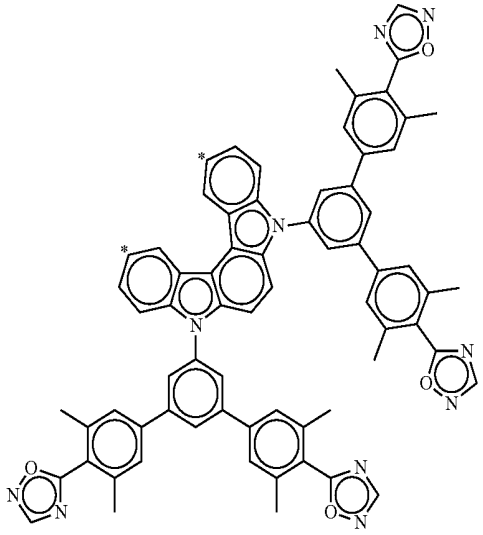
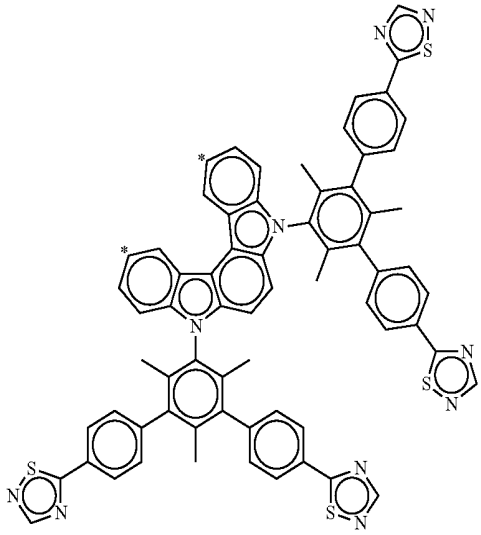
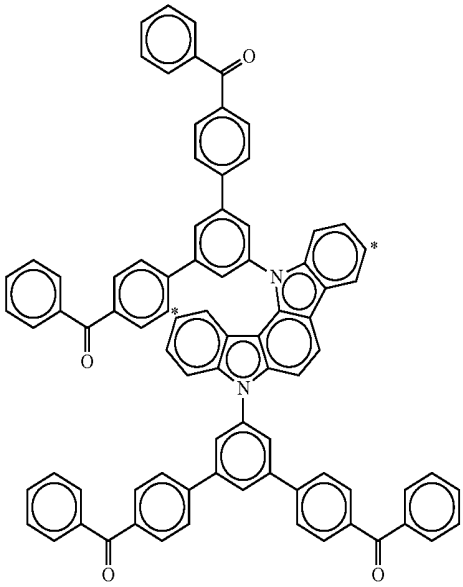


TABLE R-continued

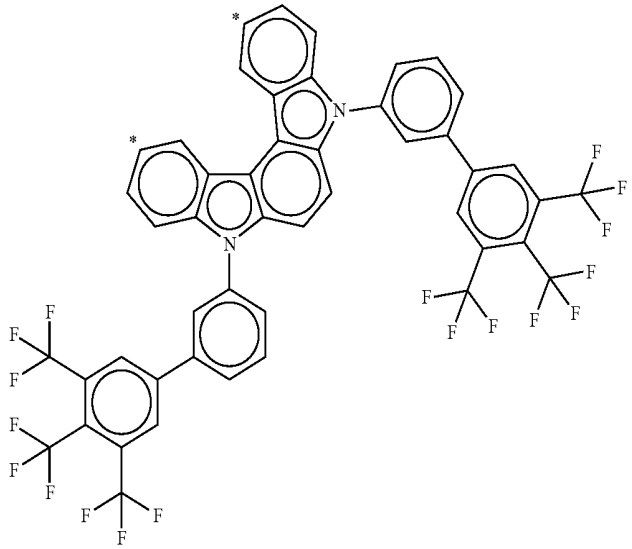
R43



R44



R45



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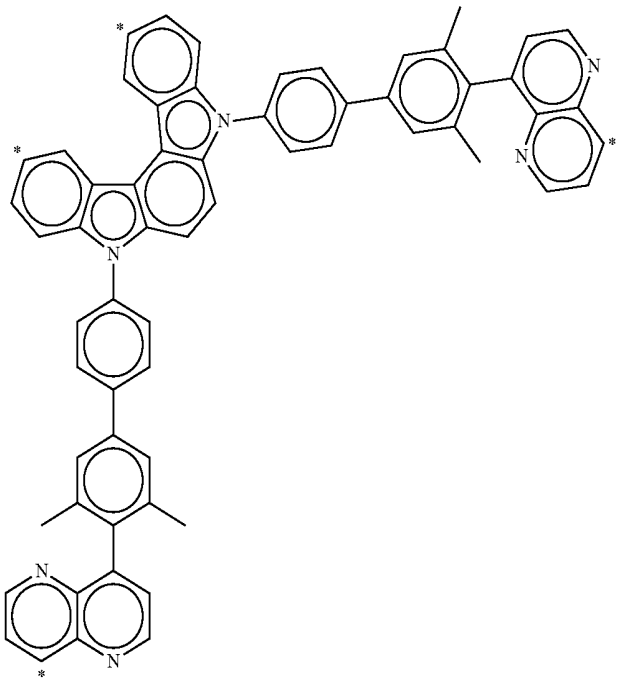
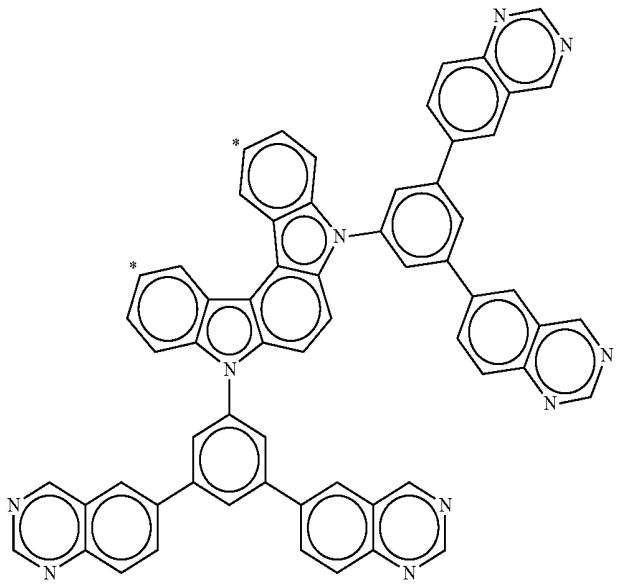
R46



R47



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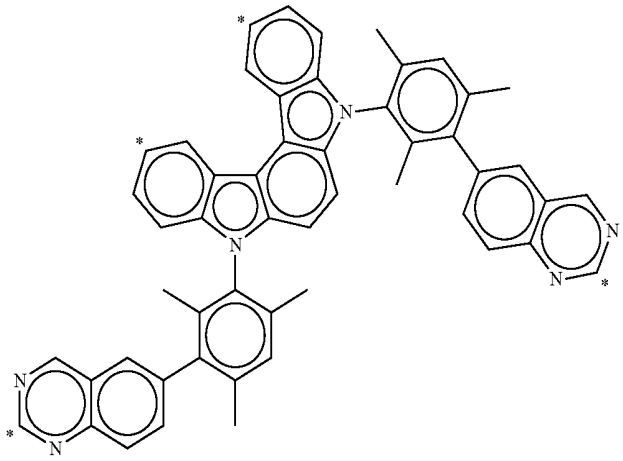
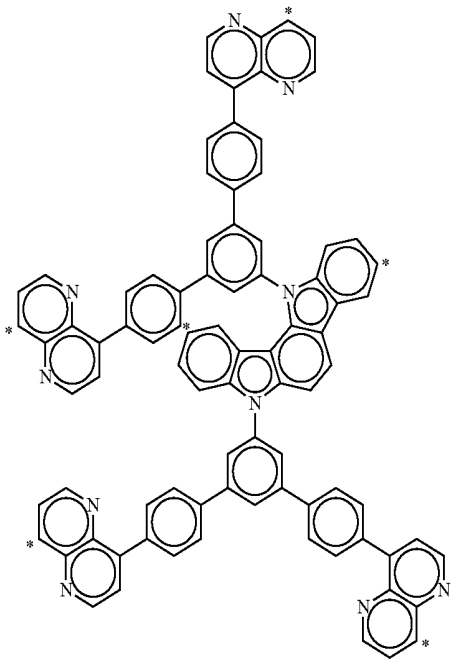
R48



R49



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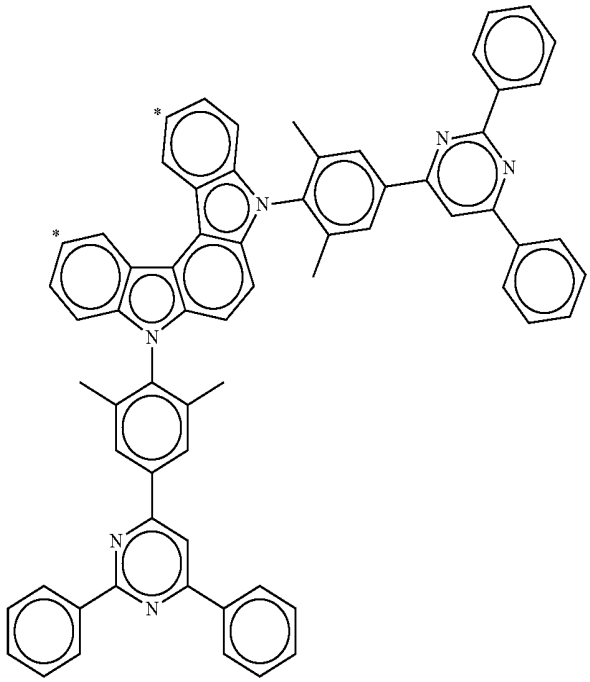
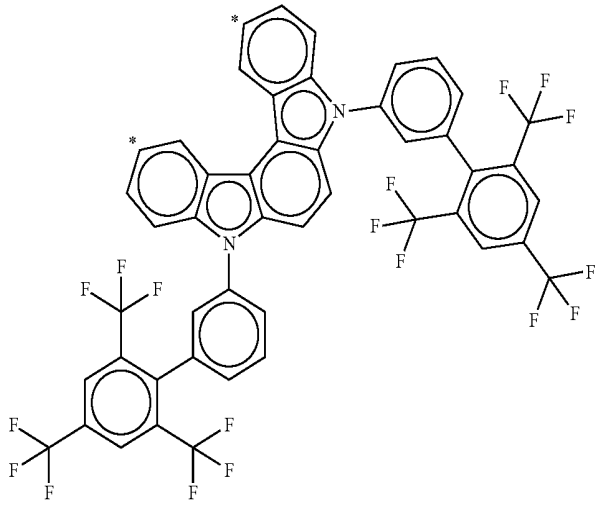
R50



R51



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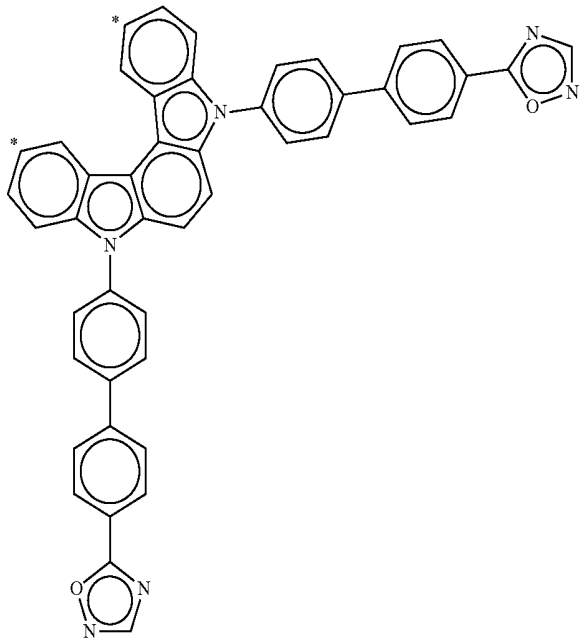
R52



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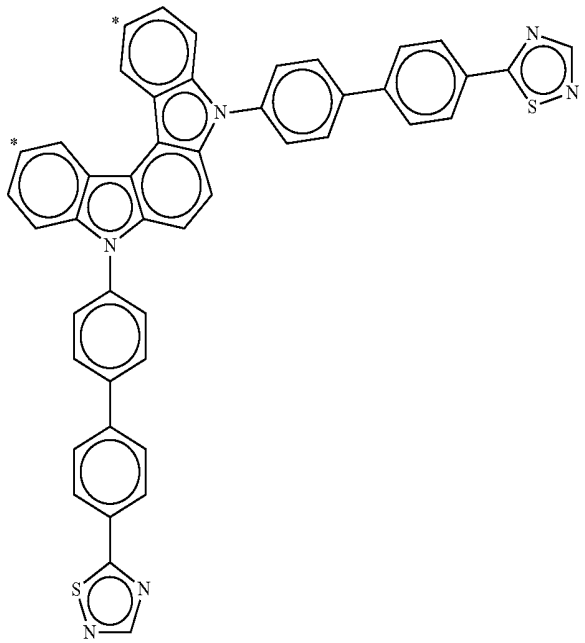

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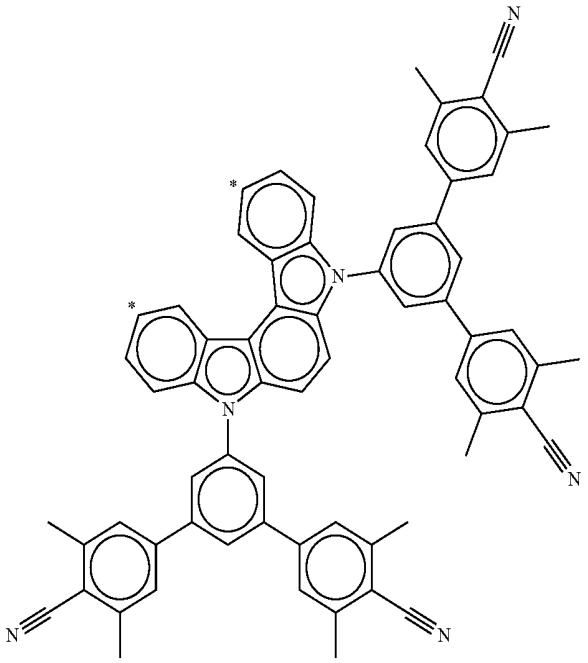
R54



R55

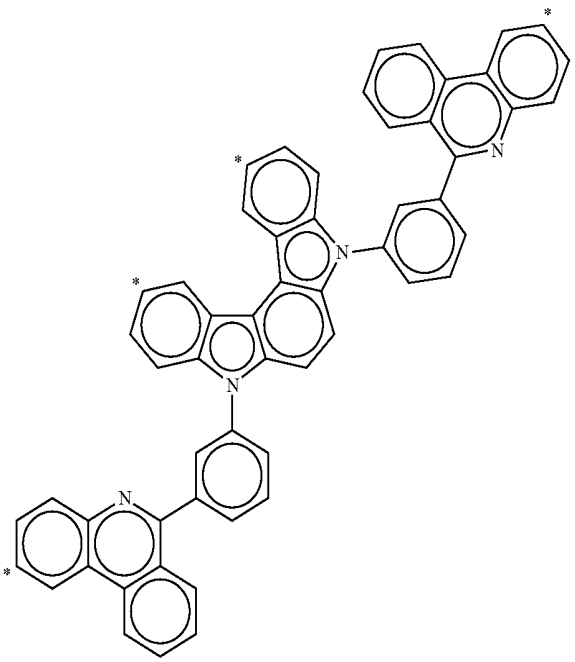
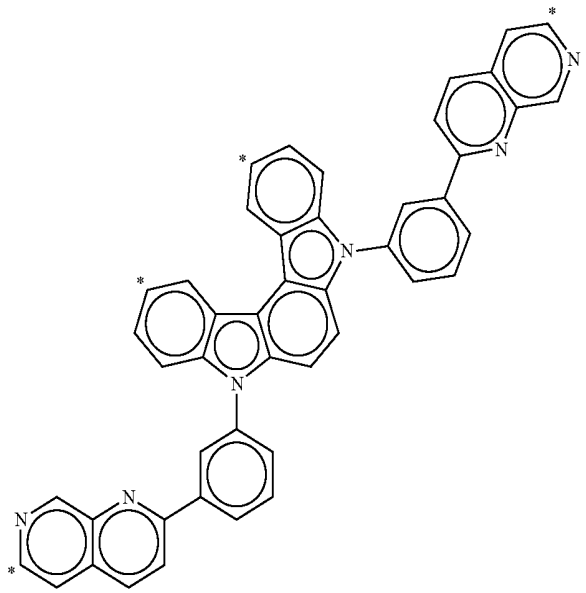
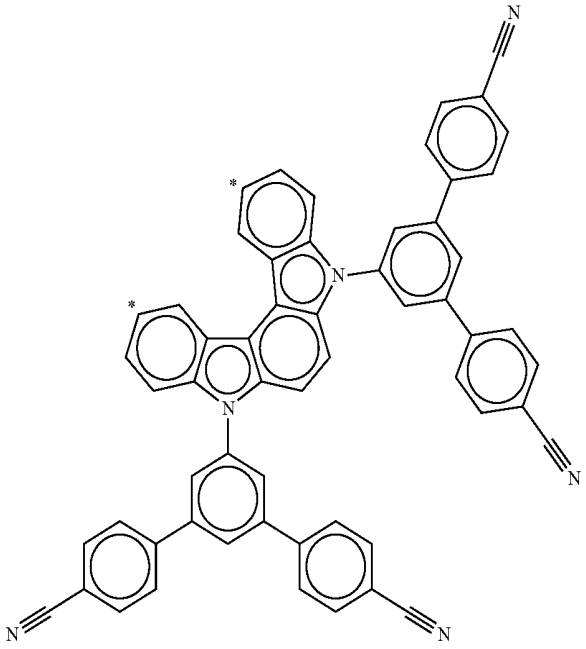


TABLE R-continued

R56



R57



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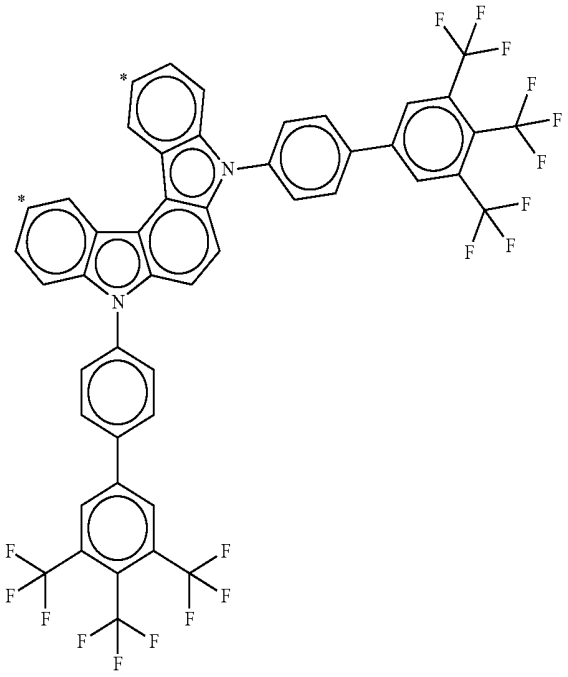
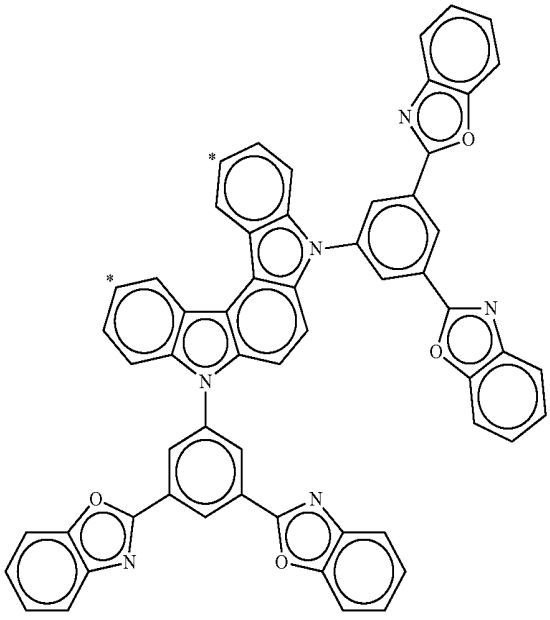
R58



R59



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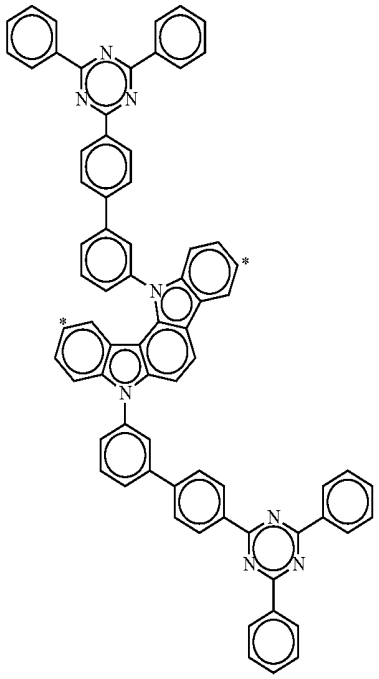
R60



R61

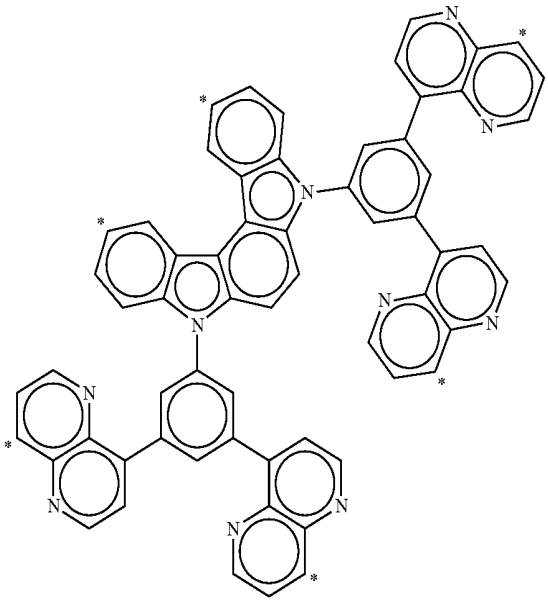
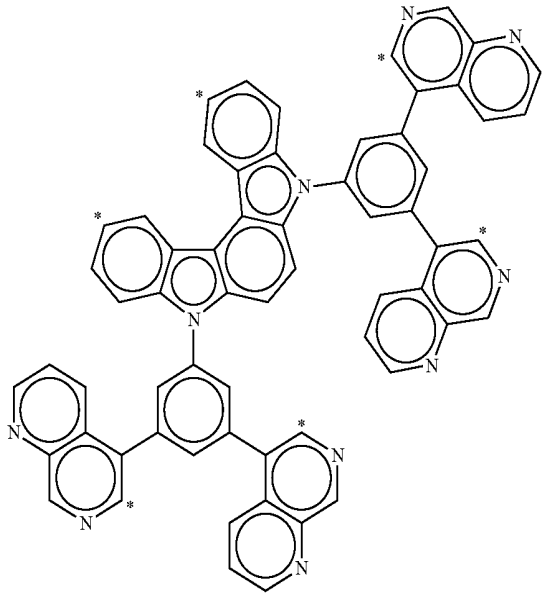


TABLE R-continued

R62



R63

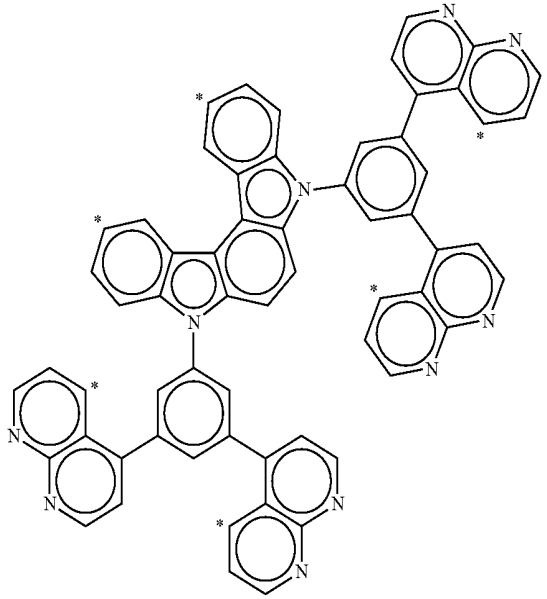
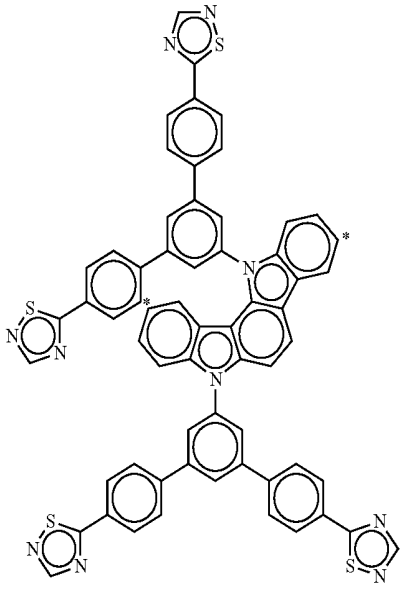


TABLE R-continued

R64



R65

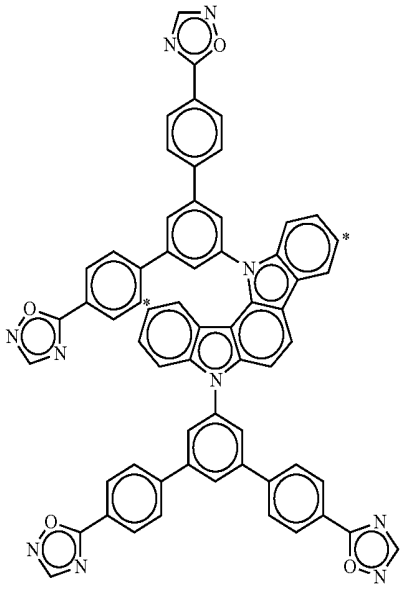
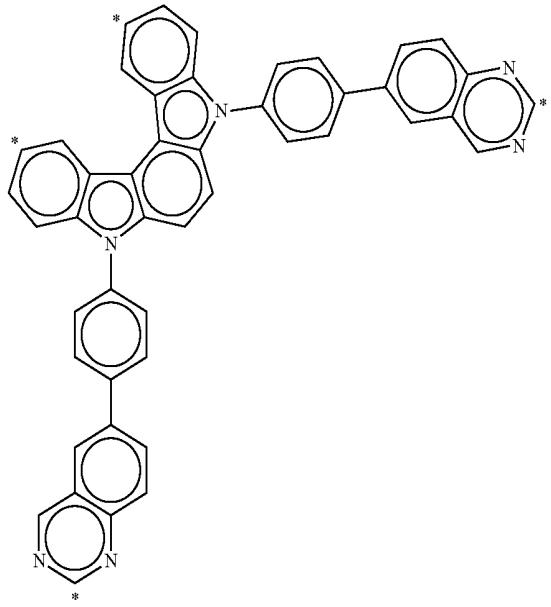
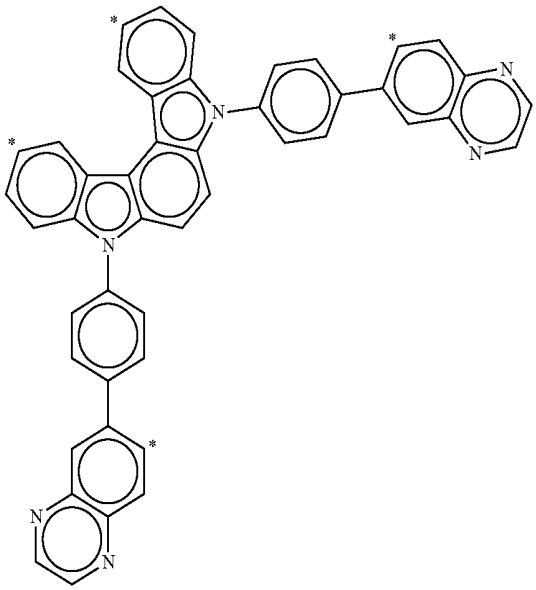


TABLE R-continued

R66



R67



R68

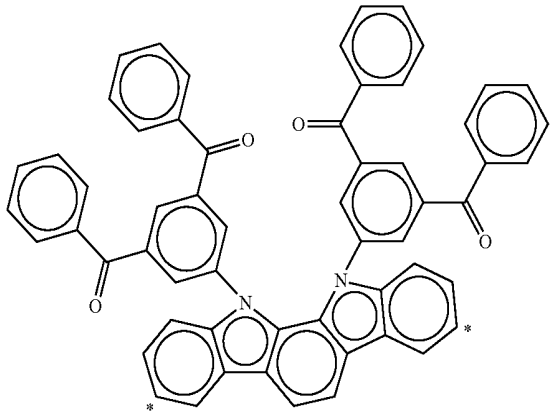
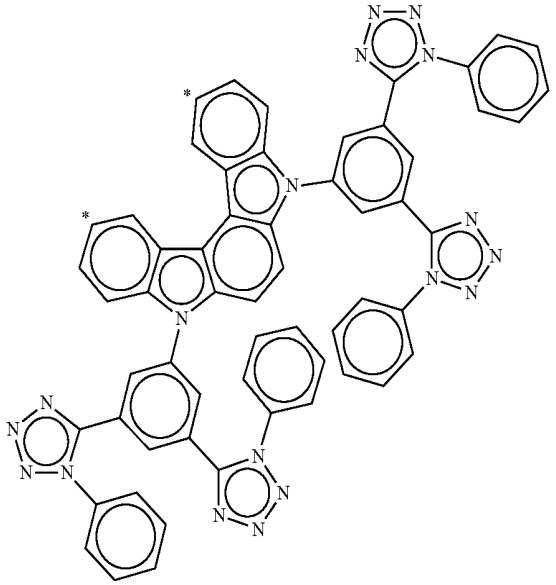
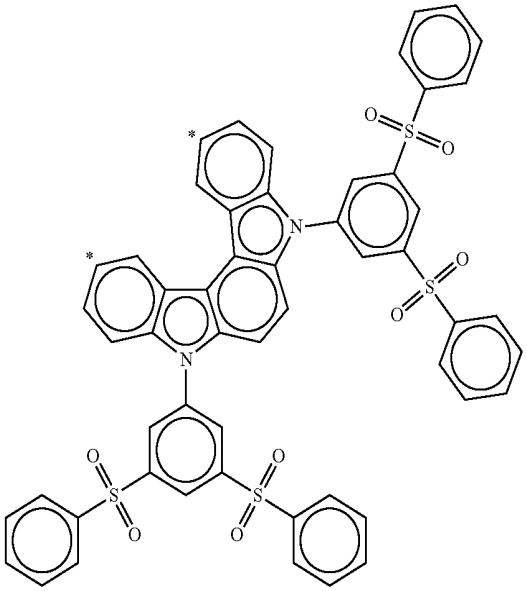


TABLE R-continued

R69



R70



R71

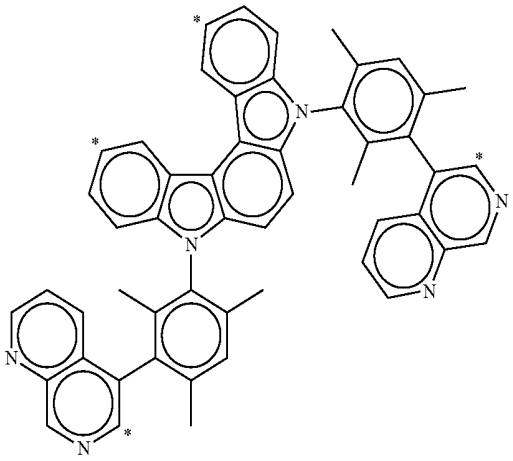
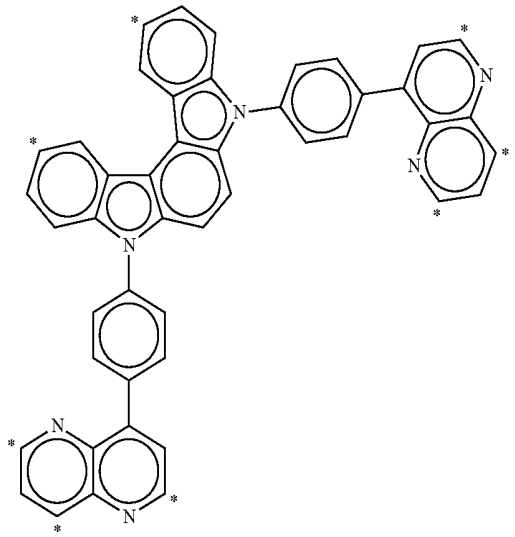
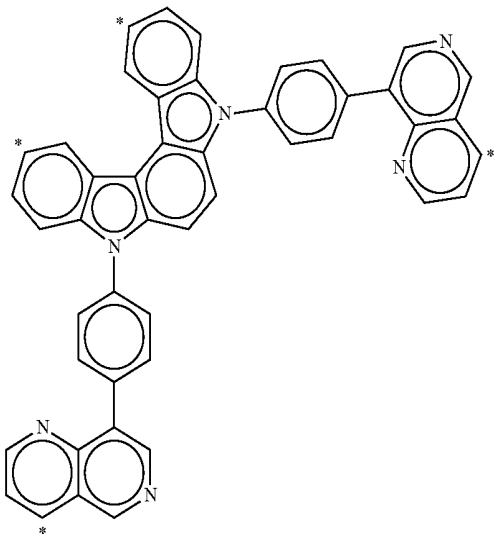


TABLE R-continued

R72



R73



R74

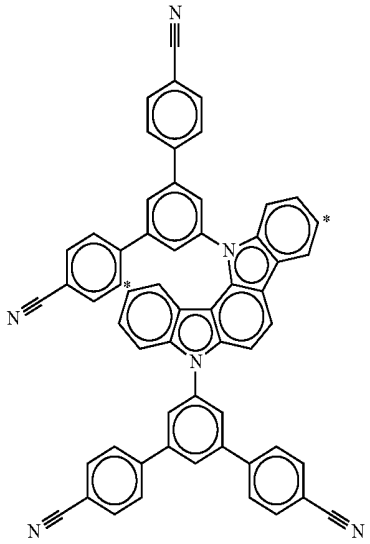
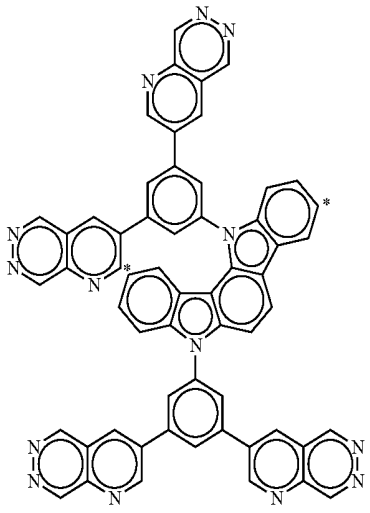


TABLE R-continued

R75



R76

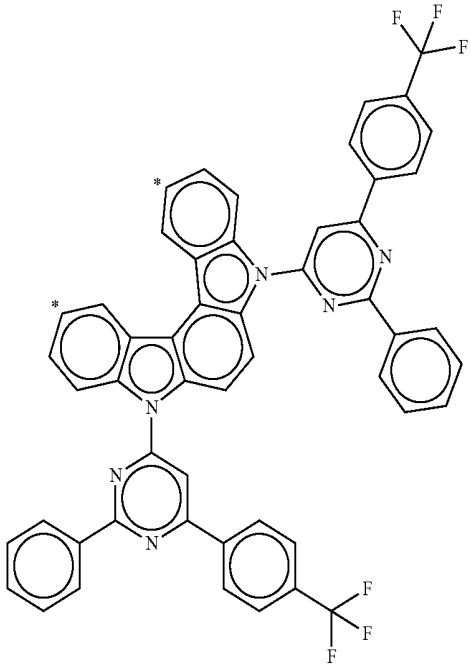
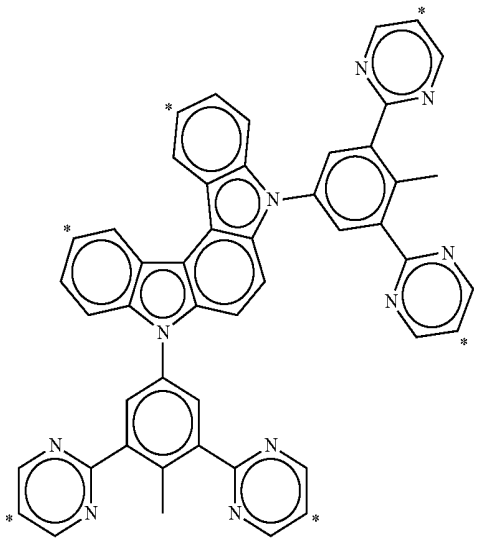
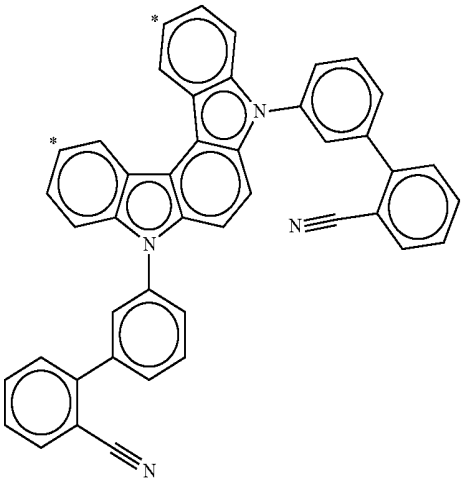


TABLE R-continued

R77



R78



R79

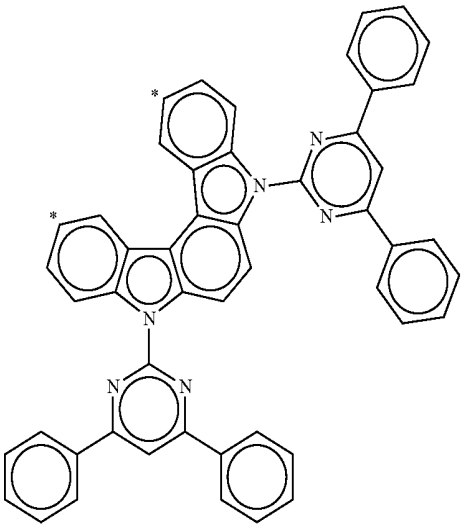
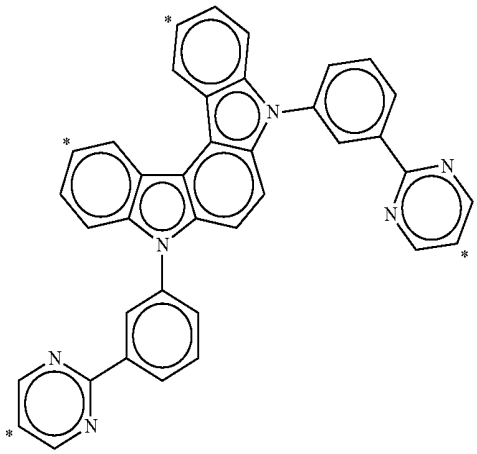
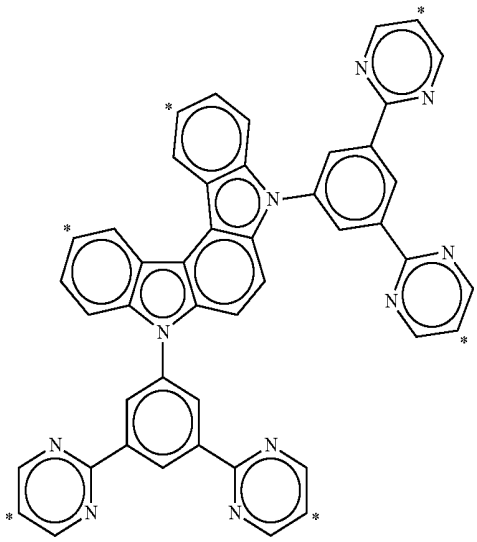


TABLE R-continued

R80



R81



R82

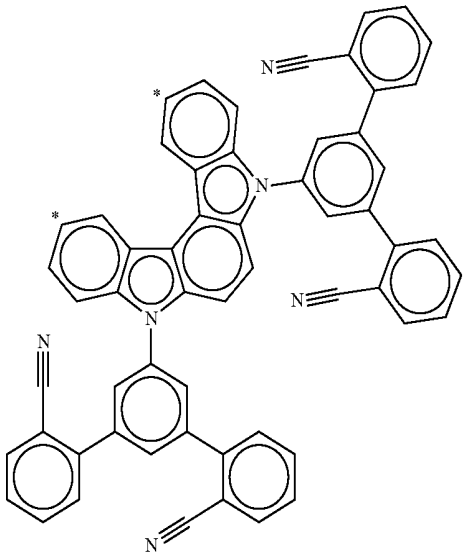
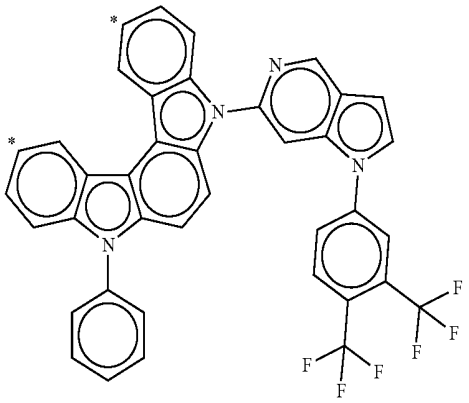
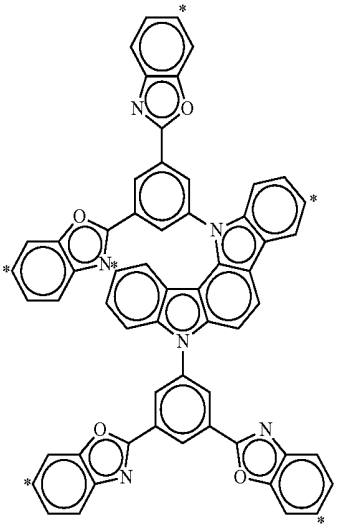


TABLE R-continued

R83



R84



R85

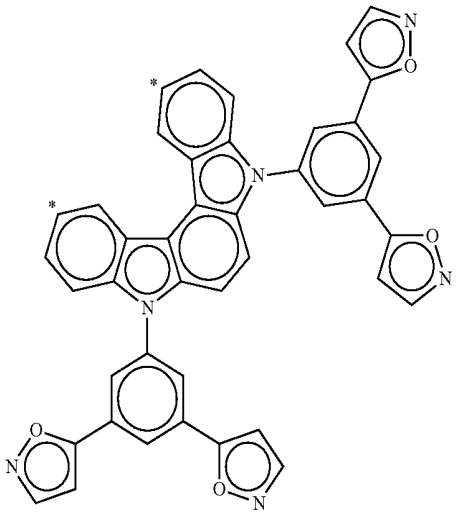
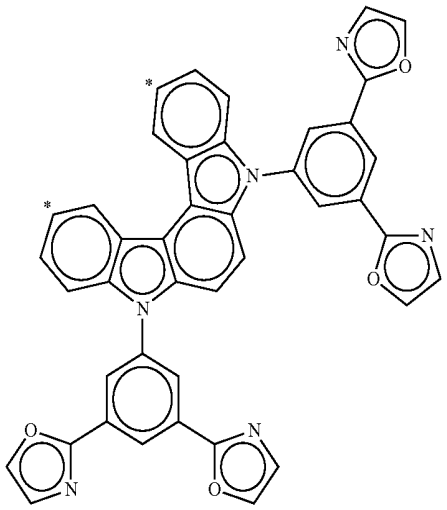
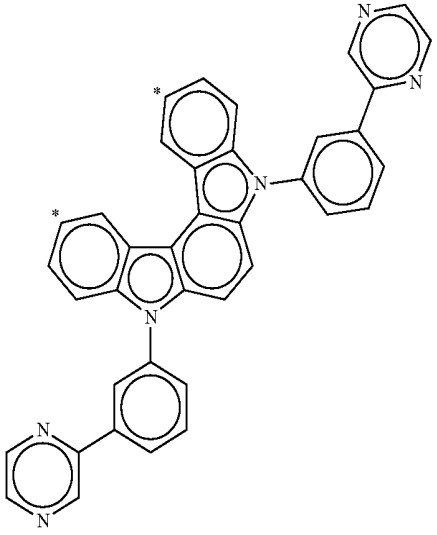


TABLE R-continued

R86



R87



R88

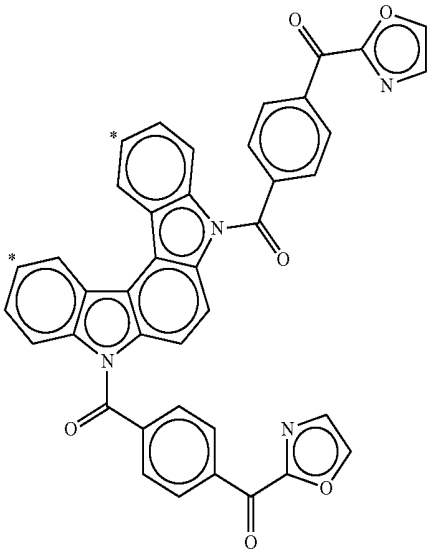
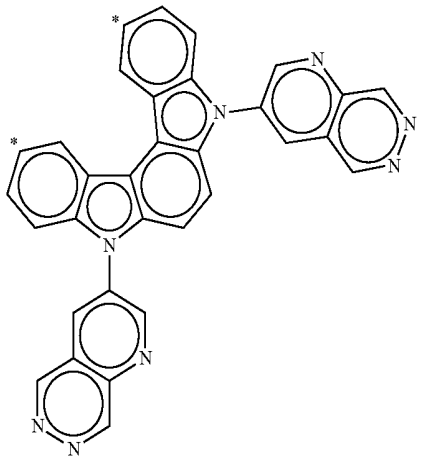
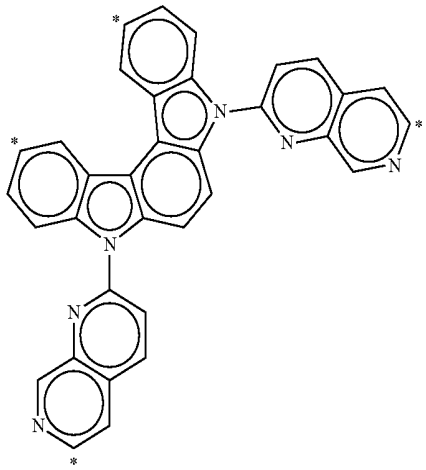


TABLE R-continued

R89



R90



R91

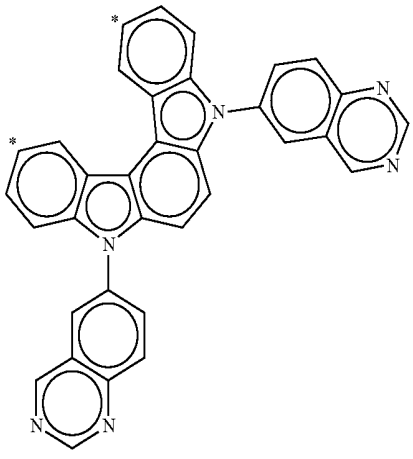
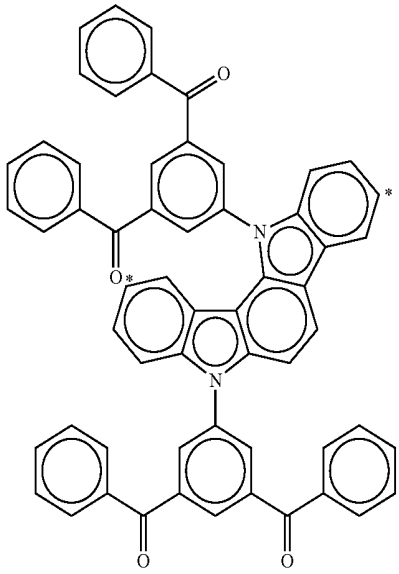
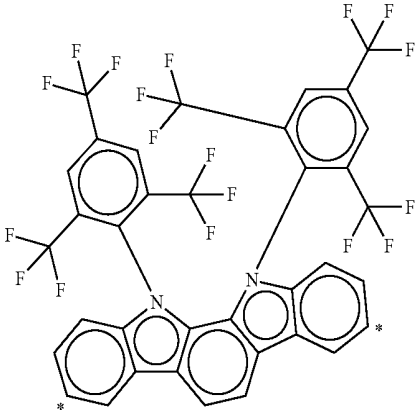


TABLE R-continued

R92



R93



R94

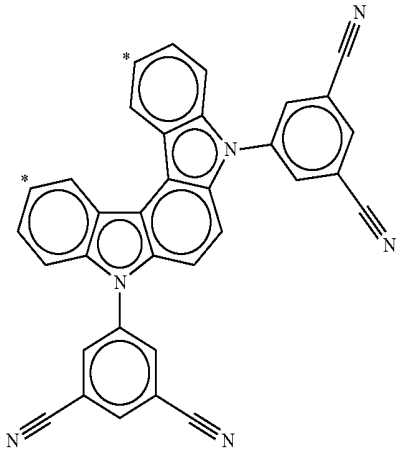
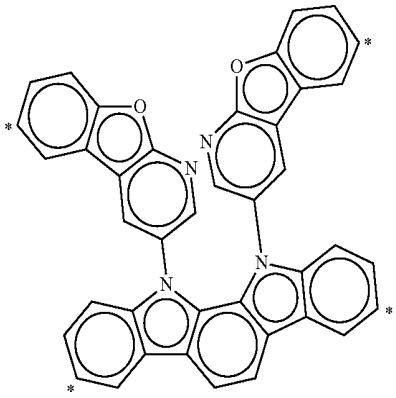
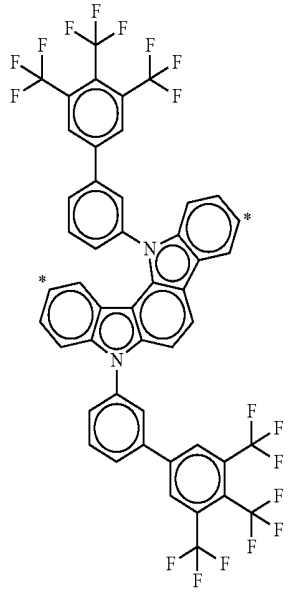


TABLE R-continued

R95



R96



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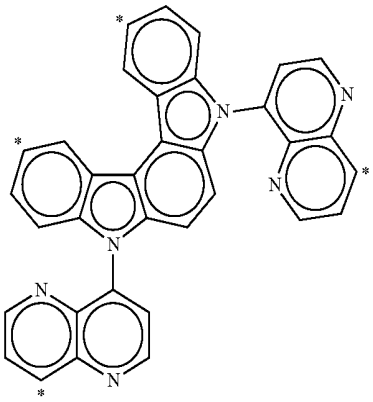

TABLE R-continued

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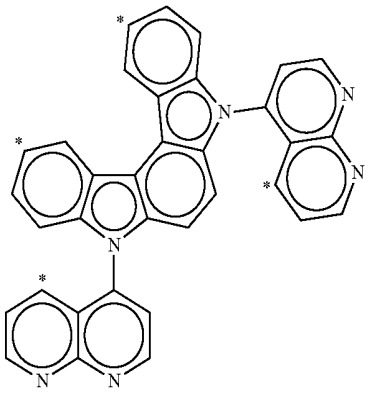
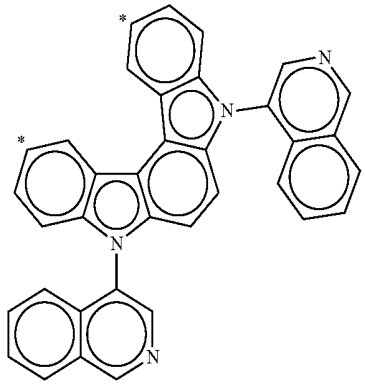


R99



R100

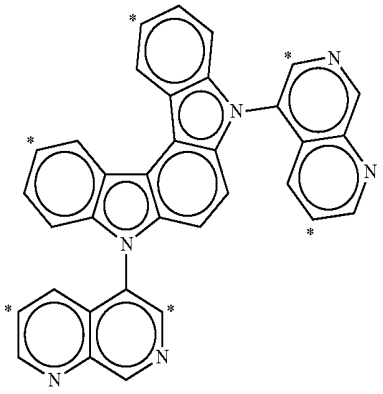
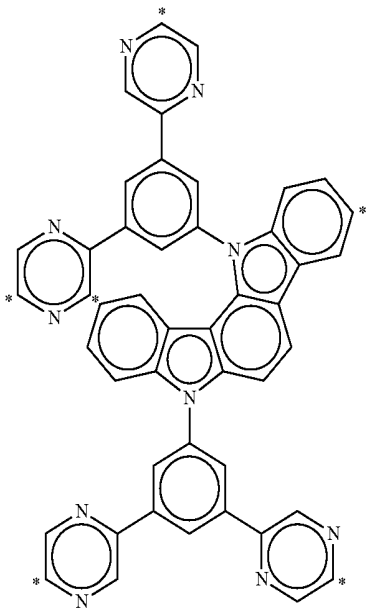


TABLE R-continued

R101



R102

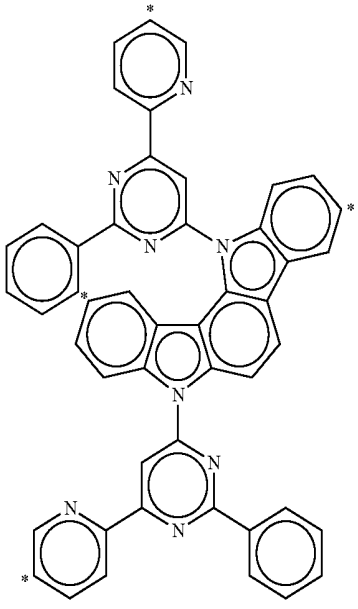
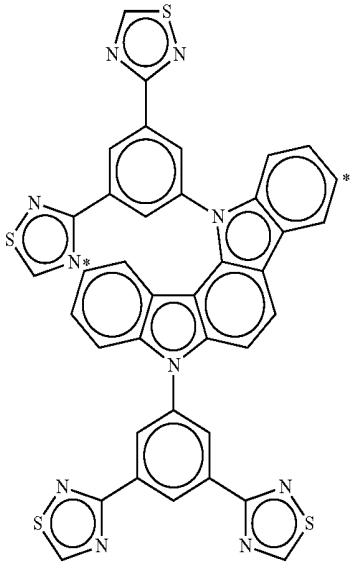
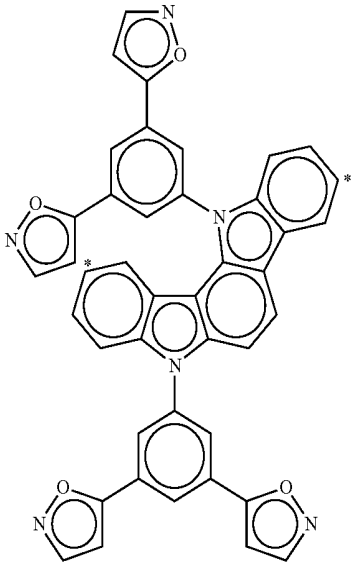


TABLE R-continued

R103



R104



R105

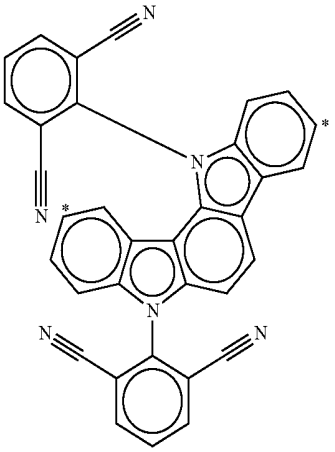
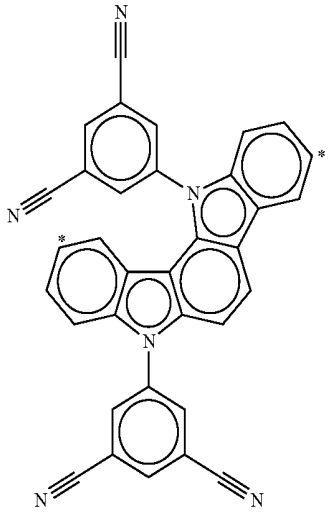


TABLE R-continued

R106



R107

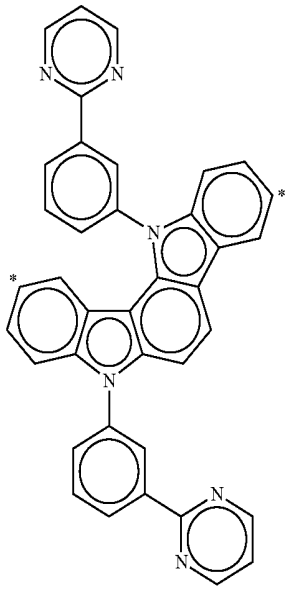
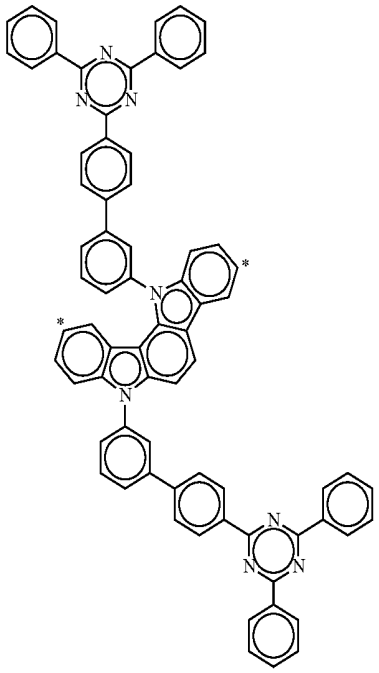


TABLE R-continued

R108



R109

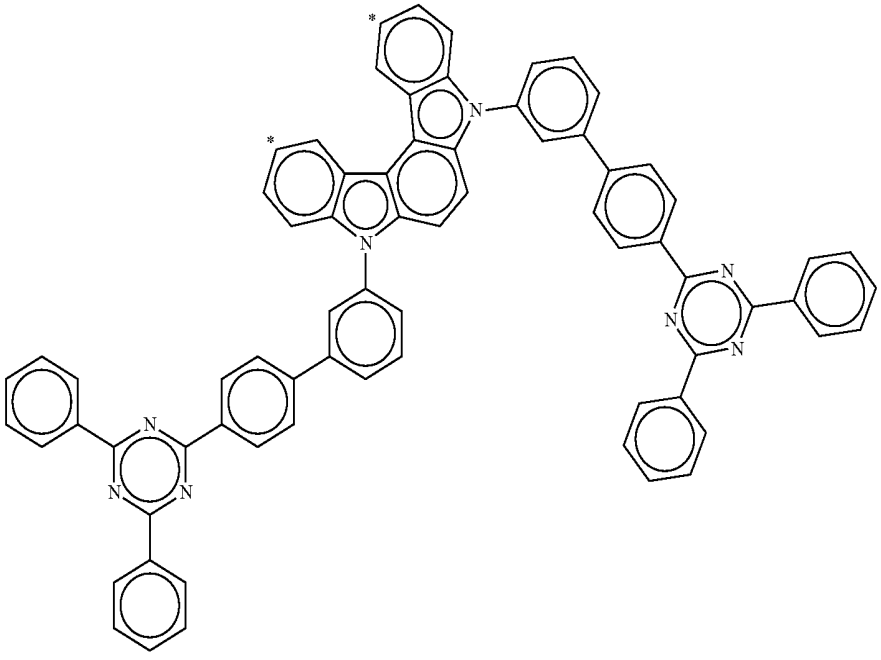
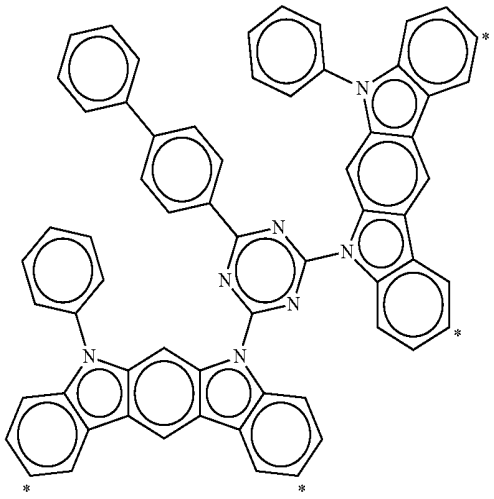


TABLE R-continued

R110	

[0193] In example embodiments of the fourteenth aspect, the invention is any one compound selected from Table R'. As described above with respect to the fourteenth aspect, in some embodiments, any substitutable carbon in the molecule is optionally substituted by R^C. In some embodiments, at least one substitutable carbon in the molecule is substituted by R^C. In some embodiments, atoms indicated by * are optionally substituted by R^C. In some embodiments, at least one atom indicated by * is substituted by R^C. In some embodiments, the molecule is not substituted, and is represented by the structural formula as depicted. The variables may be selected as described above with respect to the fourteenth aspect.

TABLE R'

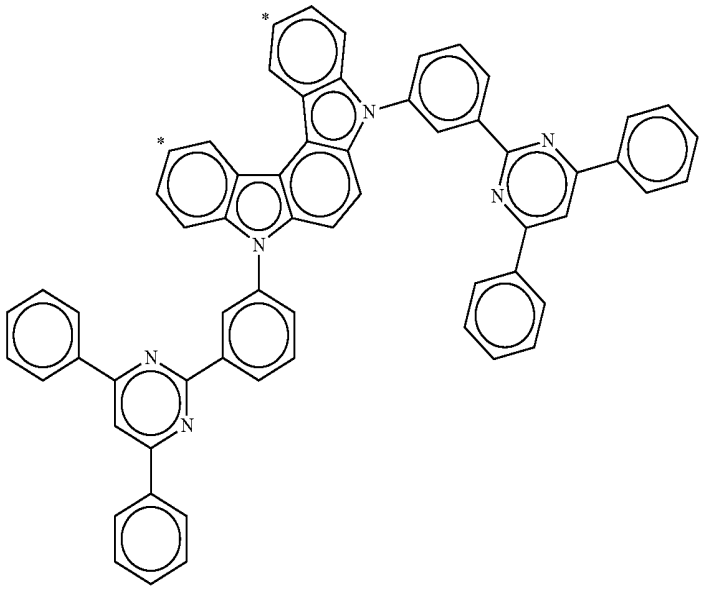
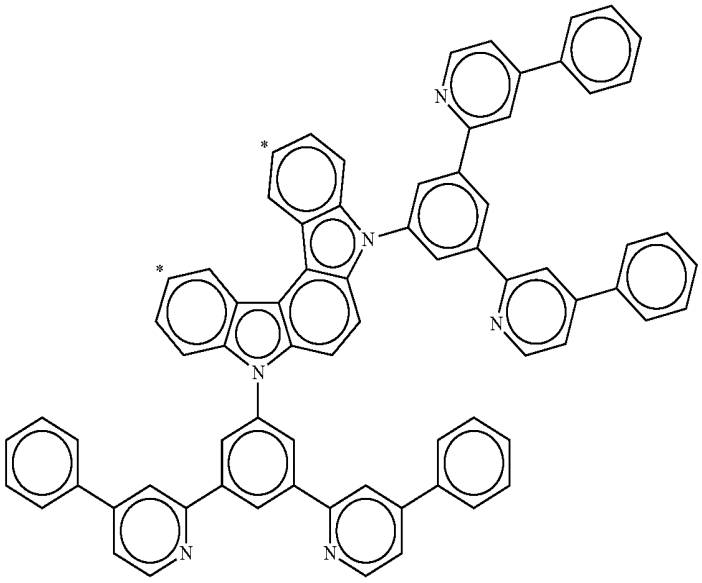
R19	

TABLE R'-continued

R20



R18

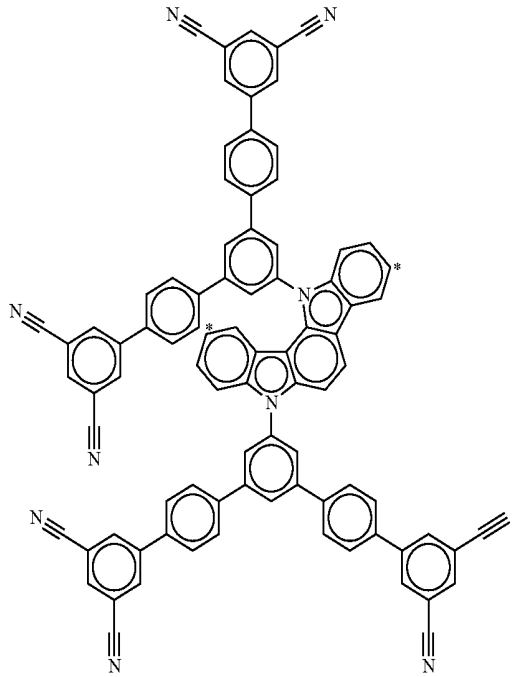
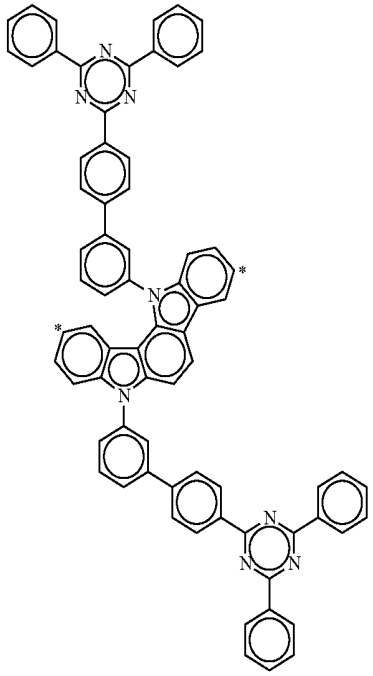


TABLE R'-continued

R108



R109

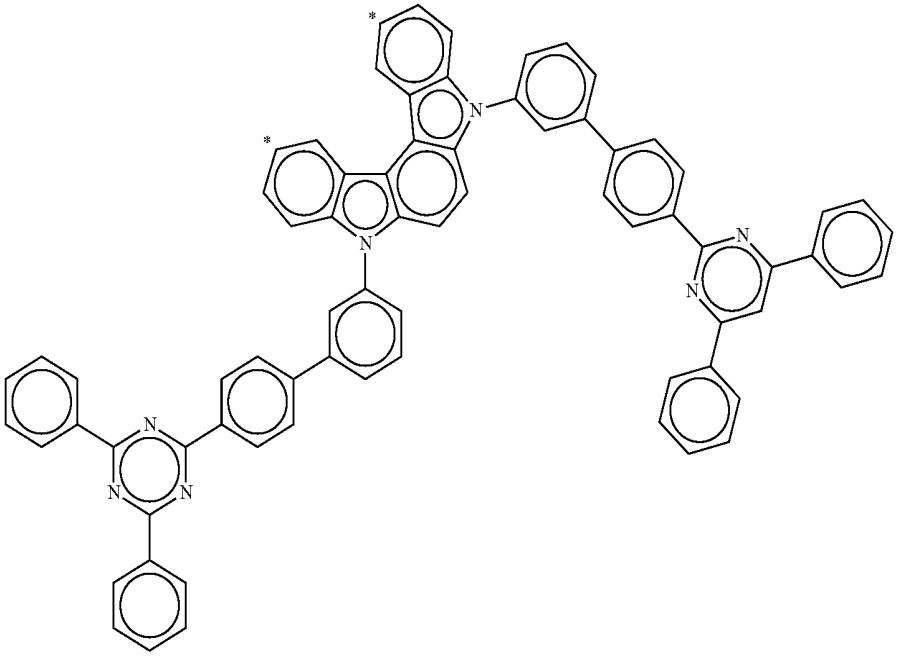
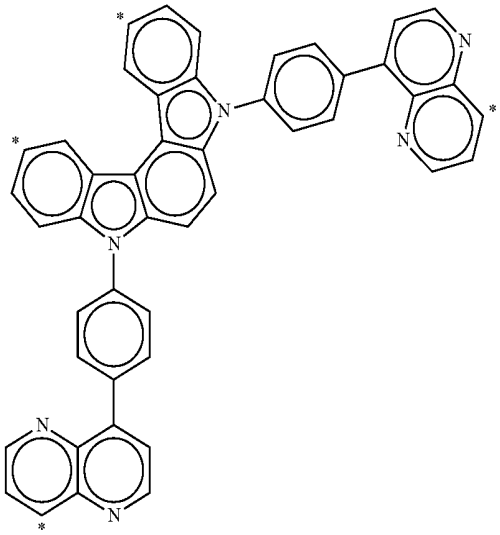


TABLE R'-continued

R72



R82

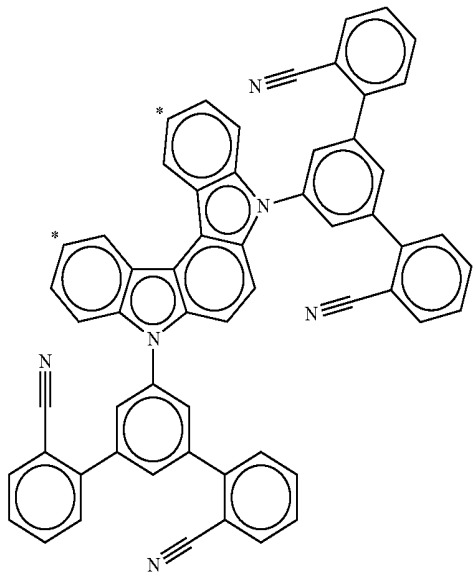
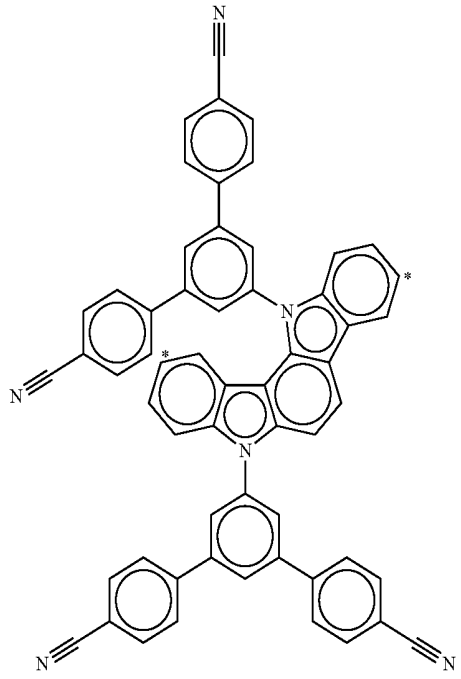


TABLE R'-continued

R74



R57

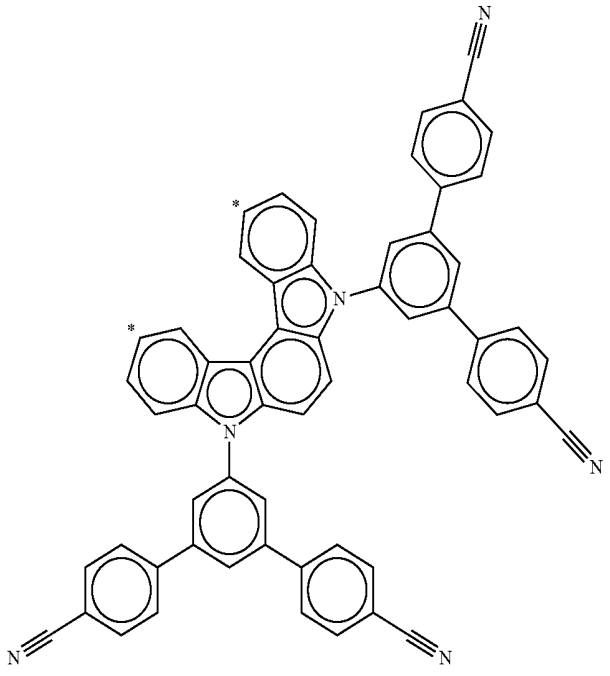
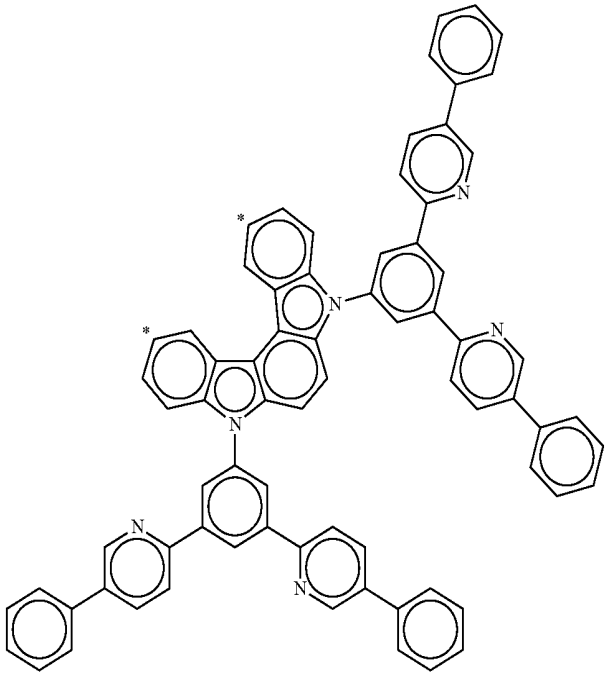


TABLE R'-continued

R38



R50

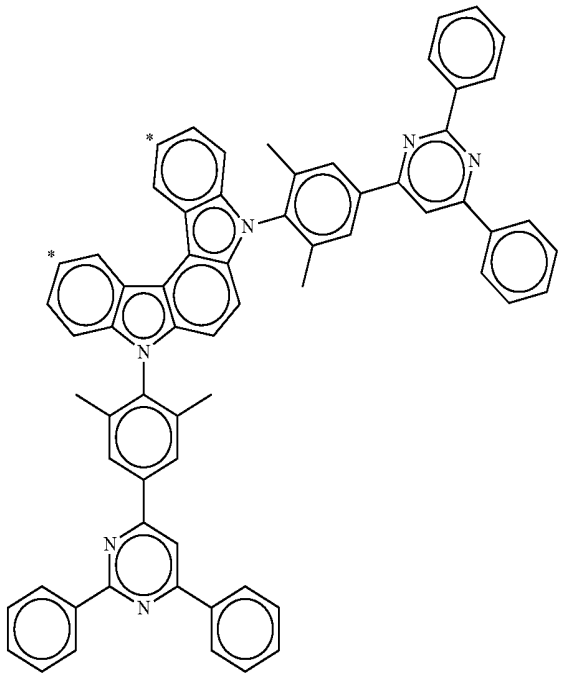
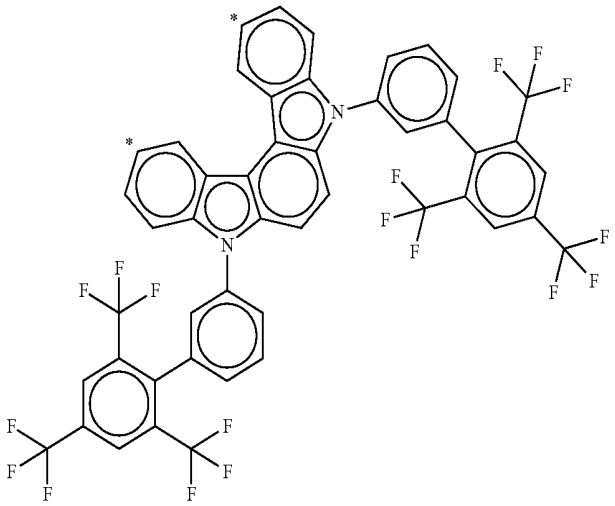
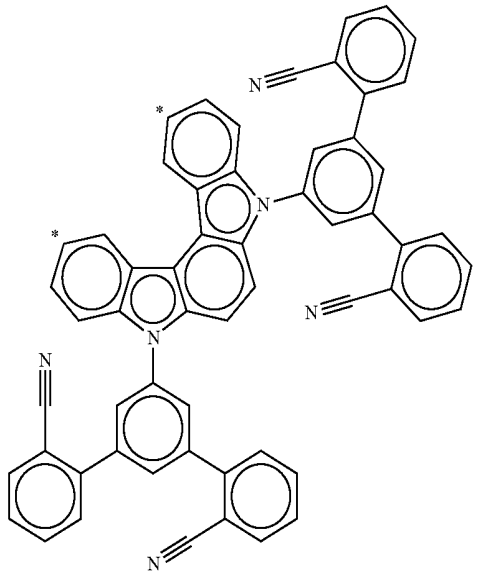


TABLE R'-continued

R51



R82



R110

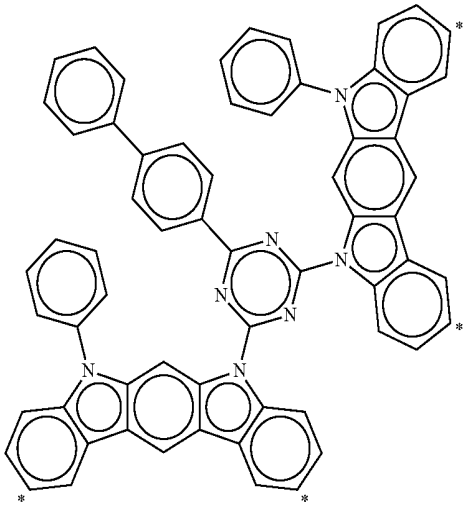
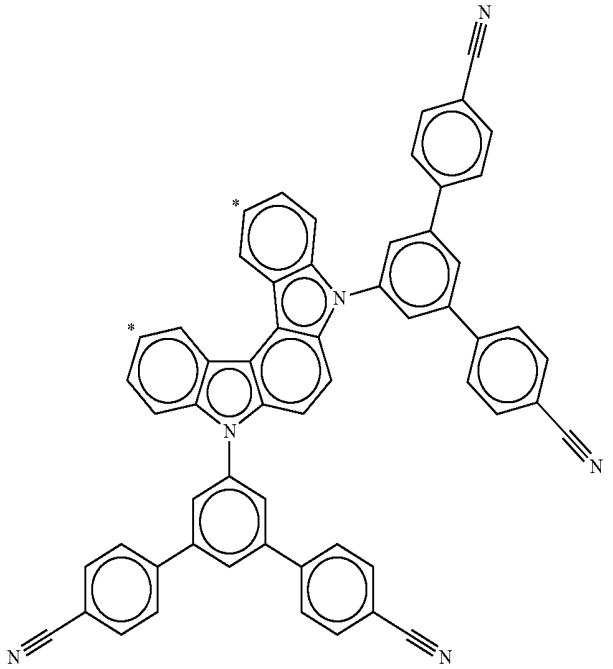
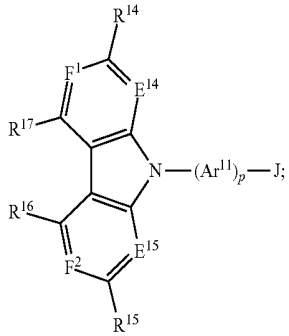


TABLE R'-continued

	R57

[0194] In a fifteenth aspect, the present invention is a molecule represented by structural formula (I):

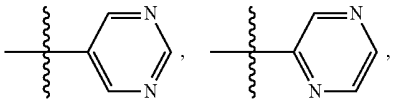


(I)

wherein:

[0195] E^{14}, and E^{15}, are, each independently, CR^A or N, wherein R^A, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0196] J is any moiety selected from —CN,



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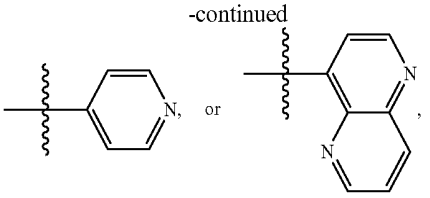


and is optionally substituted with one or more R^{11}, each independently selected from C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0197] R^{14}, R^{15}, R^{16}, and R^{17} *are*, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0198] F^1 is C—$(Ar^{12})_q$-G;

[0199] F^2 is CR^B or N, wherein R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{18}aryl, a 5-20 atom heteroaryl, a halo, or —CN, or —$(Ar^{12})_q$-G;

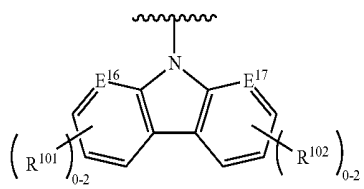
[0200] Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0201] Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0202] p is 0, 1, or 2;

[0203] q is 0 or 1; and

[0204] G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



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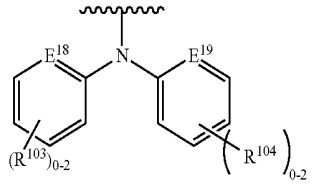


[0205] wherein:

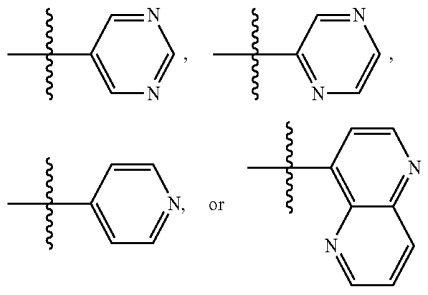
[0206] E^{16}, E^{17}, E^{18}, and E^{19} are, each independently, CR^C or N, wherein R^C is H, a C_1-C_3 alkyl, halo, or —CN; and

[0207] R101, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

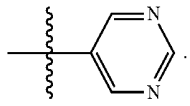
[0208] In certain embodiments of the fifteenth aspect, the molecule is not represented by any molecule represented by a structural formula in Table NN1. In certain embodiments of the fifteenth aspect, the molecule is not represented by any molecule represented by a structural formula in Table NN1, wherein the carbon or heteroatom denoted by (*) is unsubstituted or substituted by a C_1-C_6 alkyl, —OH, —CN, a halo, a C_6-C_12 aryl, a 5-20 atom heteroaryl, $—N(R^{19})_2$, or $—N(R^{20})_2$, wherein each R^{19}, independently, is H or a C_1-C_6 alkyl, or a C_5-C_{12} cycloalkyl, and wherein each R^{20}, independently, is H or a C_6-C_{18} aryl.

[0209] In certain embodiments of the fifteenth aspect, E^{14}, and E^{15} are, each independently, CR^A or N. In certain embodiments, E^{14} is CR^A. In certain embodiments, E^{14} is N. In certain embodiments, E^{15} is CR^A. In certain embodiments, E^{15} is N. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

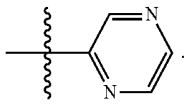
[0210] In certain embodiments of the fifteenth aspect, J is any moiety selected from —CN,



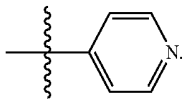
and is optionally substituted with one or more R^{11}. In certain embodiments, J is unsubstituted. In certain embodiments, J is —CN. In certain embodiments, J is



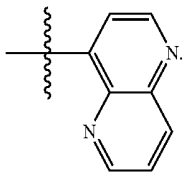
In certain embodiments, J is



In certain embodiments, J is



In certain embodiments, J is



The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0211] In certain embodiments of the fifteenth aspect, each R^{11} is independently selected from C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each R^{11} is independently selected from C_1-C_6 alkyl or C_6-C_{18} aryl. In certain embodiments, each R^{11} is independently selected from C_1-C_6 alkyl or phenyl. In certain embodiments, each R^{11} is independently selected from C_1-C_3 alkyl or phenyl. In certain embodiments, each R^{11} is independently selected from methyl or phenyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0212] In certain embodiments of the fifteenth aspect, R^{14} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{14} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{14} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{14} is H or methyl. In certain embodiments, R^{14} is H. In certain embodiments, R^{14} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{14} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{14} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{14} is methyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0213] In certain embodiments of the fifteenth aspect, R^{15} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{15} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{15} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{15} is H or methyl. In certain embodiments, R^{15} is H. In certain embodiments, R^{15} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{15} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a

halo, or —CN. In certain embodiments, R^{15} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{15} is methyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

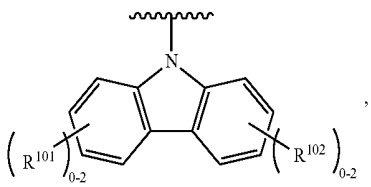
[0214] In certain embodiments of the fifteenth aspect, R^{16} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{16} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{16} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{16} is H or methyl. In certain embodiments, R^{16} is H. In certain embodiments, R^{16} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{16} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{16} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{16} is methyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0215] In certain embodiments of the fifteenth aspect, R^{17} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{17} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{17} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{16} is H or methyl. In certain embodiments, R^{17} is H. In certain embodiments, R^{17} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{17} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{17} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{17} is methyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0216] In certain embodiments of the fifteenth aspect, F^1 is C—$(Ar^{12})_q$-G. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0217] In certain embodiments of the fifteenth aspect, F^2 is N or CR^B. In certain embodiments, F^2 is CR^B. In certain embodiments, F^2 is N. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0218] In certain embodiments of the fifteenth aspect, each R^B is, independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{18}aryl, a 5-20 atom heteroaryl, a halo, or —CN, or $—(Ar^{12})_q$-G. In certain embodiments, each R^B is, independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or $—(Ar^{12})_q$-G. In certain embodiments, each R^B is, independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or a moiety represented by one of the following structural formulas:



, or

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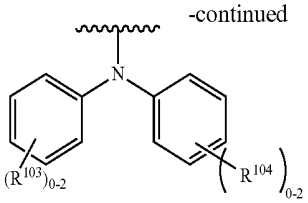
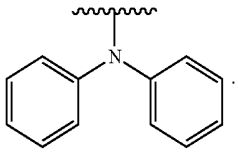
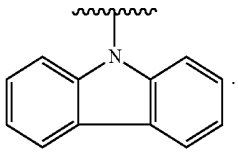


In certain embodiments, each R^B is, independently, H or a moiety represented by the following structural formula:



In certain embodiments, each R^B is, independently, H or a moiety represented by the following structural formula:



The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

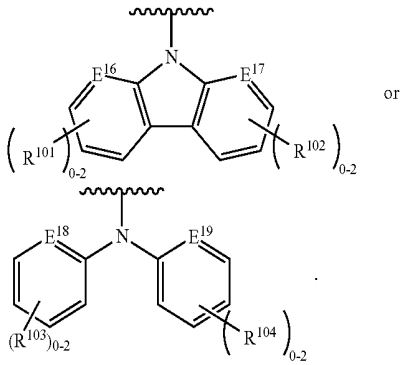
[0219] In certain embodiments of the fifteenth aspect, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four methyls. In certain embodiments, Ar^{11}, for each occurrence, is unsubstituted phenyl. In certain embodiments, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_2-C_6 alkyls. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0220] In certain embodiments of the fifteenth aspect, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four methyls. In certain embodiments, Ar^{12}, for each occurrence, is unsubstituted phenyl. In certain embodiments, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_2-C_6 alkyls. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0221] In certain embodiments of the fifteenth aspect, p is 0 or 1. In certain embodiments, p is 0. In certain embodiments, p is 1. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

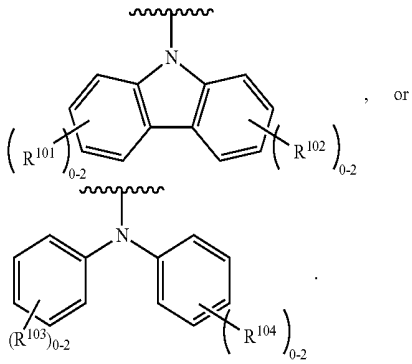
[0222] In certain embodiments of the fifteenth aspect, q is 0 or 1. In certain embodiments, q is 0. In certain embodiments, q is 1. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0223] In certain embodiments of the fifteenth aspect, G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



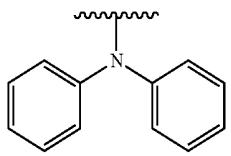
or

In certain embodiments, G is a moiety represented by one of the following structural formulas:

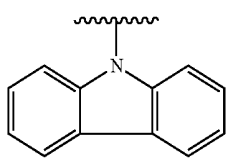


, or

In certain embodiments, G is a moiety represented the following structural formula:



In certain embodiments, G is a moiety represented the following structural formula:



The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0224] In certain embodiments of the fifteenth aspect, E^{16} is CR^C or N. In certain embodiments, E^{16} is CR^C. In certain embodiments, E^{16} is N. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0225] In certain embodiments of the fifteenth aspect, E^{17} is CR^C or N. In certain embodiments, E^{17} is CR^C. In certain embodiments, E^{17} is N. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0226] In certain embodiments of the fifteenth aspect, E^{18} is CR^C or N. In certain embodiments, E^{18} is CR^C. In certain embodiments, E^{18} is N. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0227] In certain embodiments of the fifteenth aspect, E^{19} is CR^C or N. In certain embodiments, E^{19} is CR^C. In certain embodiments, E^{19} is N. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0228] In certain embodiments of the fifteenth aspect, each R^C is, independently, H, a C_1-C_3 alkyl, halo, or —CN. In certain embodiments, each R^C is H. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0229] In certain embodiments of the fifteenth aspect, each R^{102} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments of the fifteenth aspect, each R^{102} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0230] In certain embodiments of the fifteenth aspect, each R^{102} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments of the fifteenth aspect, each R^{102} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0231] In certain embodiments of the fifteenth aspect, each R^{103} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments of the fifteenth aspect, each R^{103} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0232] In certain embodiments of the fifteenth aspect, each R^{104} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments of the fifteenth aspect, each R^{104} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0233] In certain embodiments of the fifteenth aspect:

[0234] R^A, for each occurrence independently, is H or a C_1-C_6 alkyl;

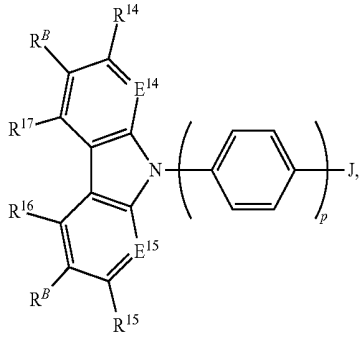
[0235] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl;

[0236] F^2 is CR^B; and

[0237] R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or $-(Ar^{12})_q$-G.

The remainder of the variables in structural formula (I) are as described above and below with respect to the fifteenth aspect.

[0238] In certain embodiments of the fifteenth aspect, the molecule is represented by the following structural formula:



wherein the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect. In certain embodiments:

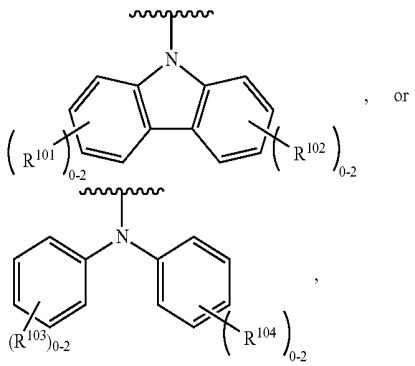
[0239] E^{14}, and E^{15}, are, each independently, CR^A or N, wherein R^A, for each occurrence independently, is H or a C_1-C_6 alkyl;

[0240] p is 0 or 1;

[0241] R^{11} is a C_6-C_{18} aryl or a 5-20 atom heteroaryl;

[0242] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN;

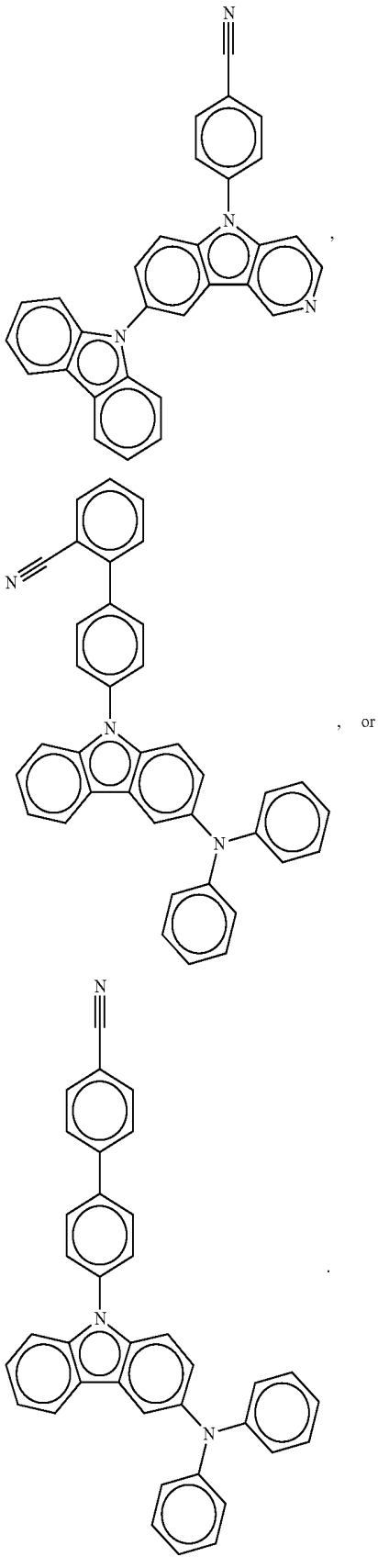
[0243] R^B is, for each occurrence independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or a moiety represented by one of the following structural formulas:



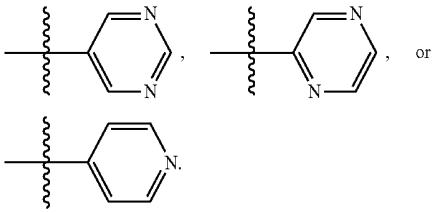
[0244] wherein:

[0245] R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl.

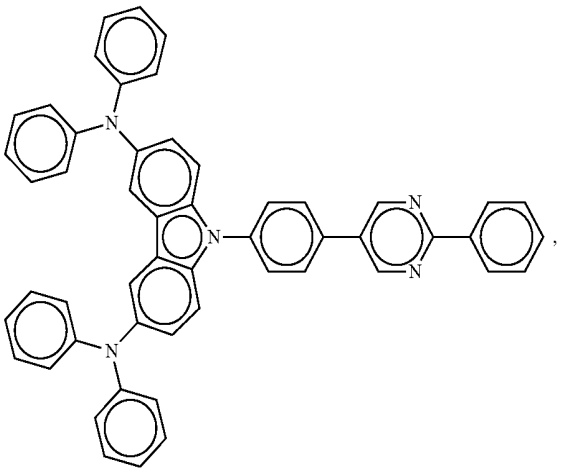
[0246] In certain embodiments of the fifteenth aspect, J is —CN. In certain embodiments, the molecule is represented by one of the following structural formulas:

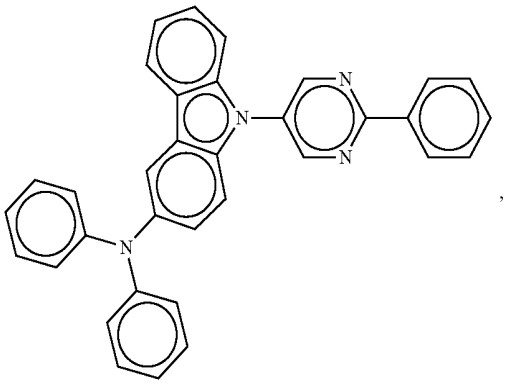


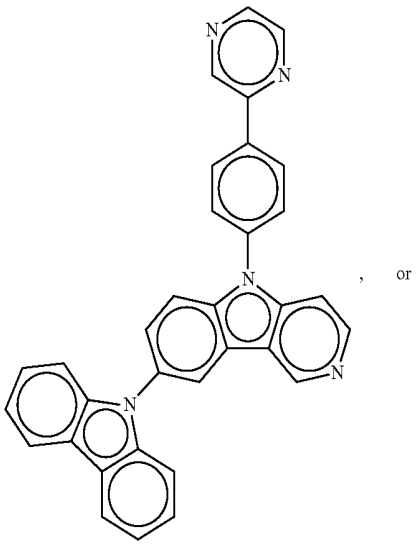
[0247] In certain embodiments of the fifteenth aspect, J is



In certain embodiments, the molecule is represented by one of the following structural formulas:







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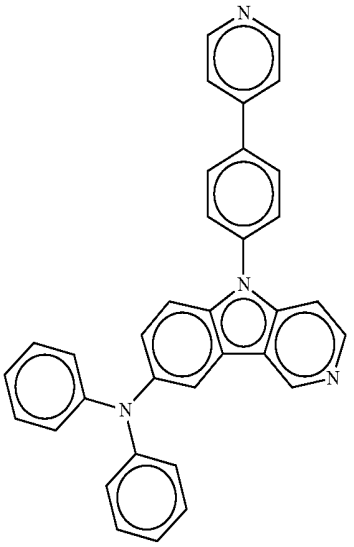
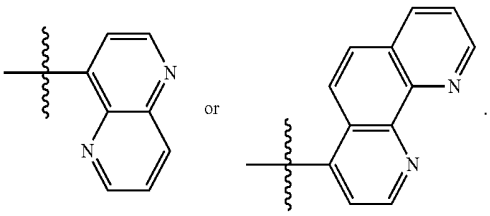
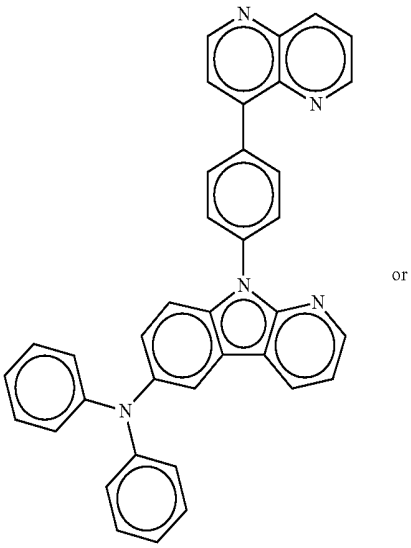


[0248] In certain embodiments of the fifteenth aspect, J is



In certain embodiments, the molecule is represented by one of the following structural formulas:



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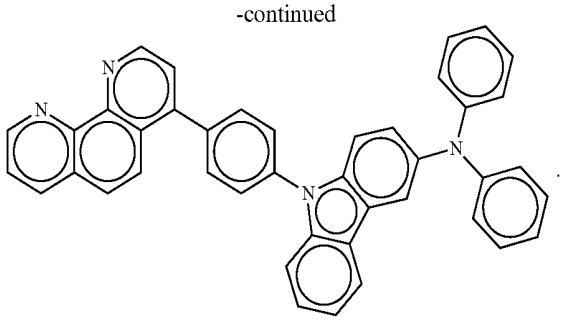
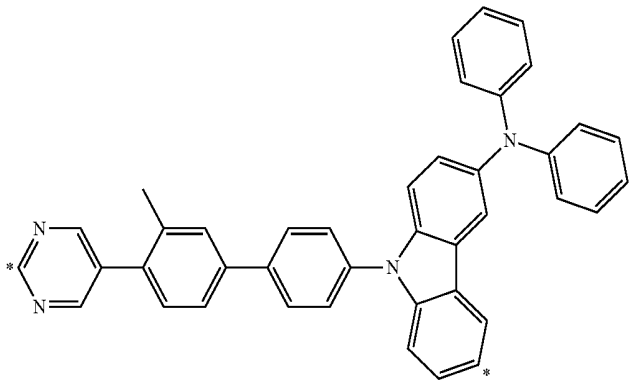
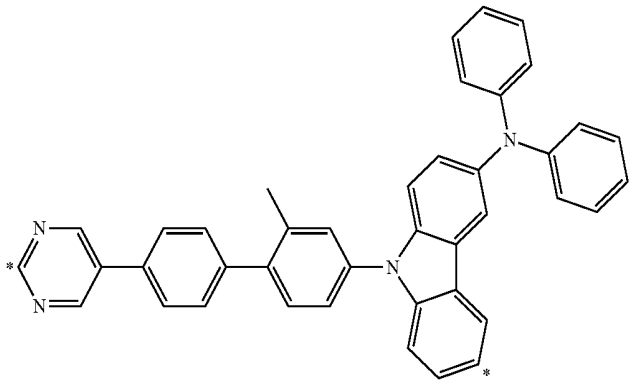


TABLE NN1





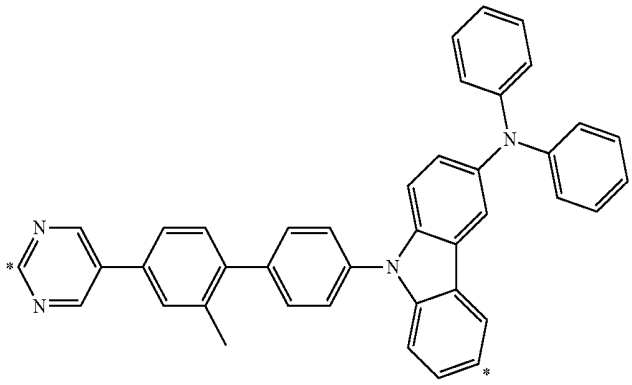
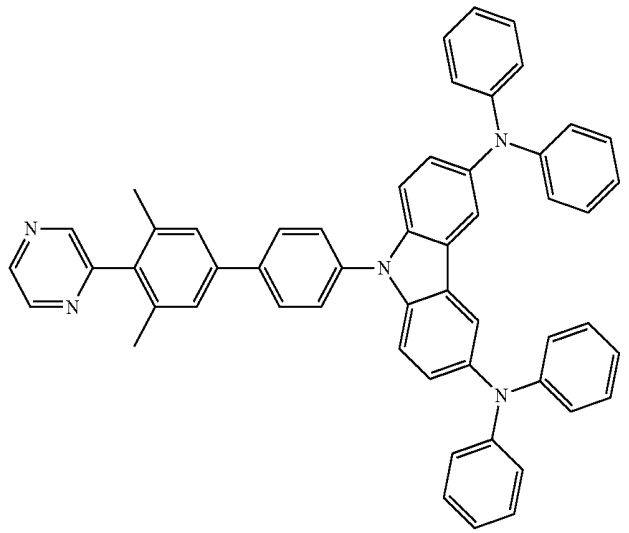
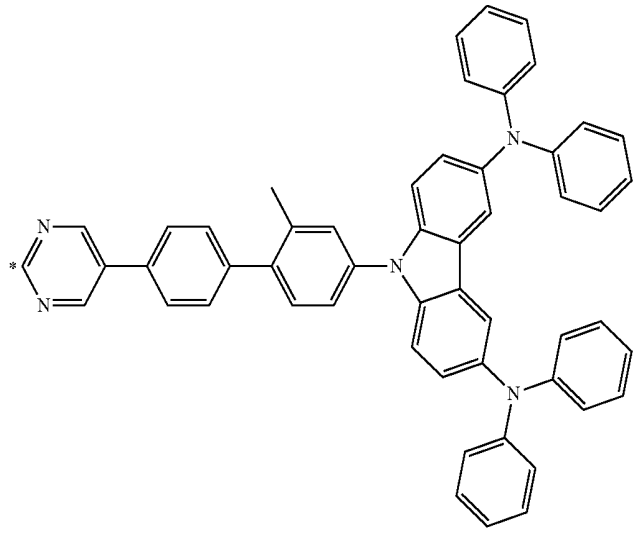


TABLE NN1-continued





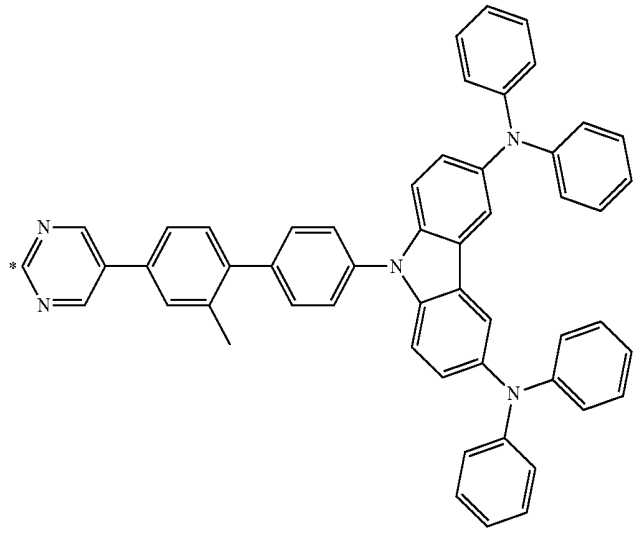
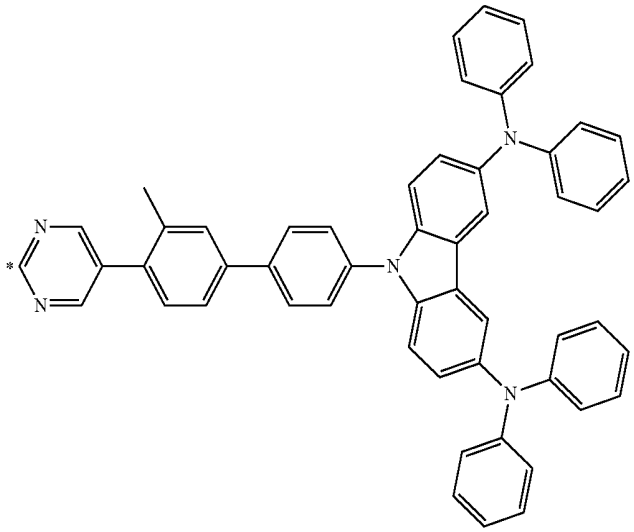
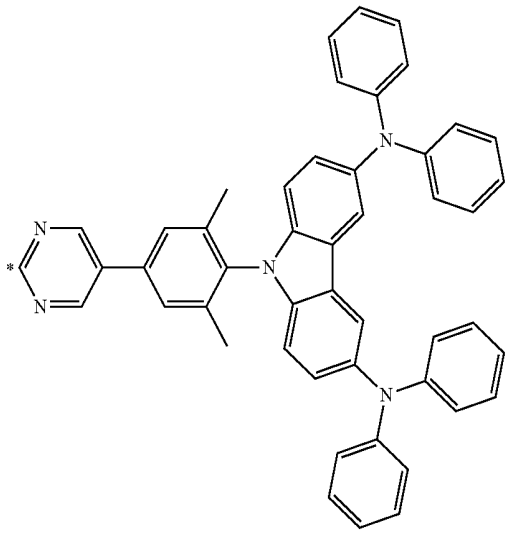


TABLE NN1-continued





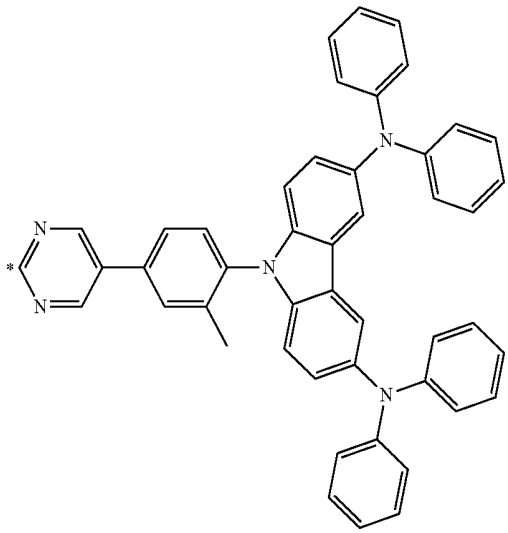
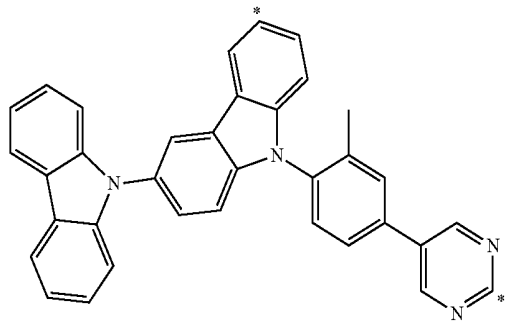
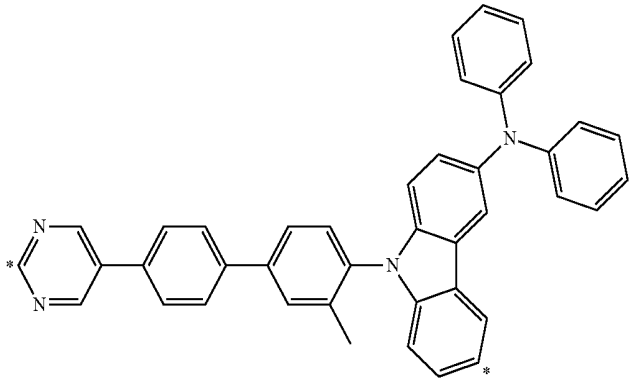
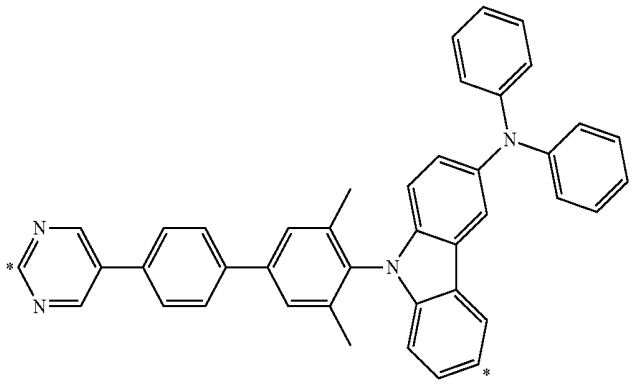


TABLE NN1-continued







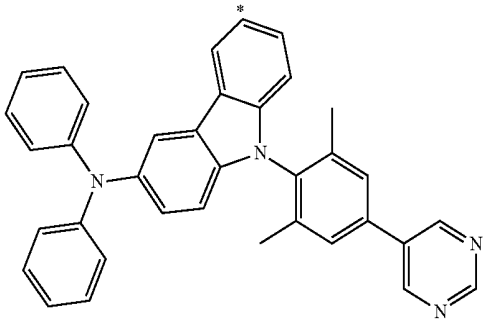
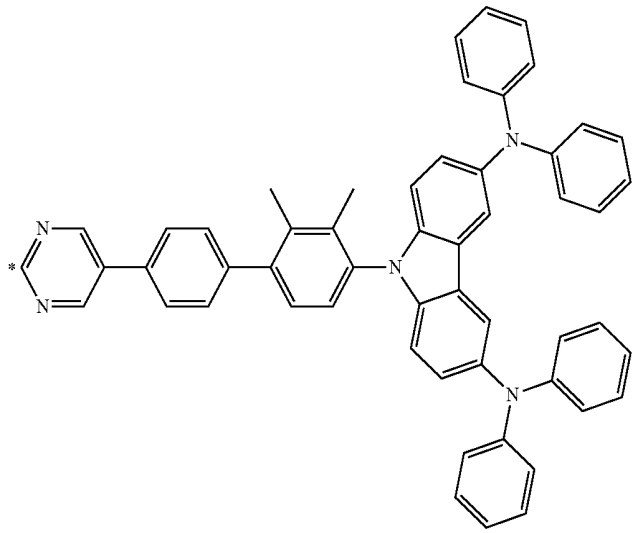
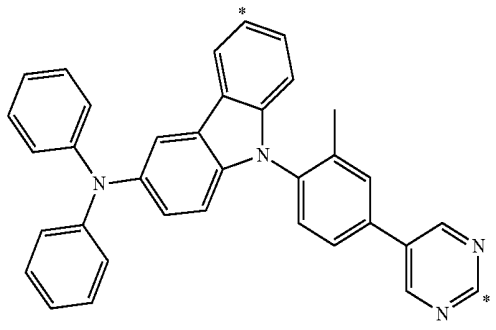
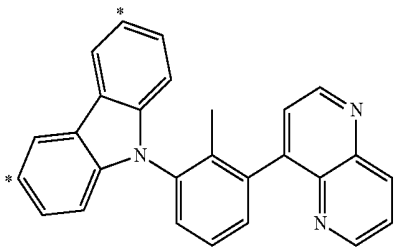


TABLE NN1-continued







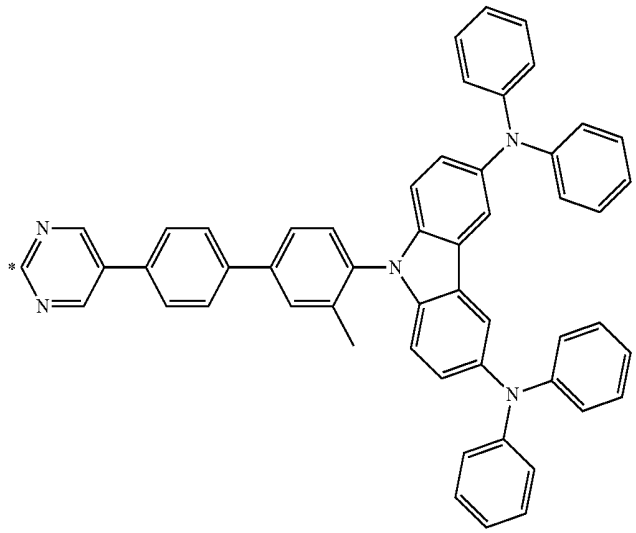
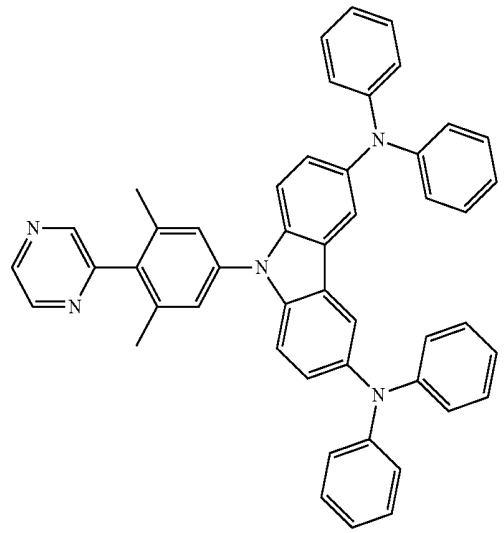
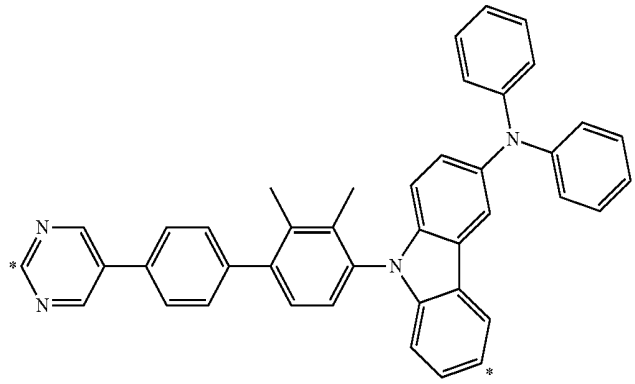


TABLE NN1-continued





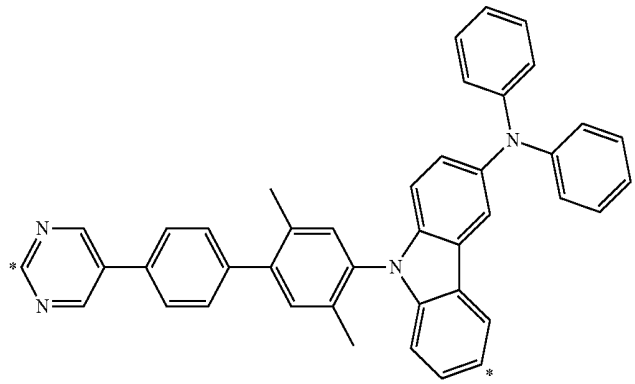
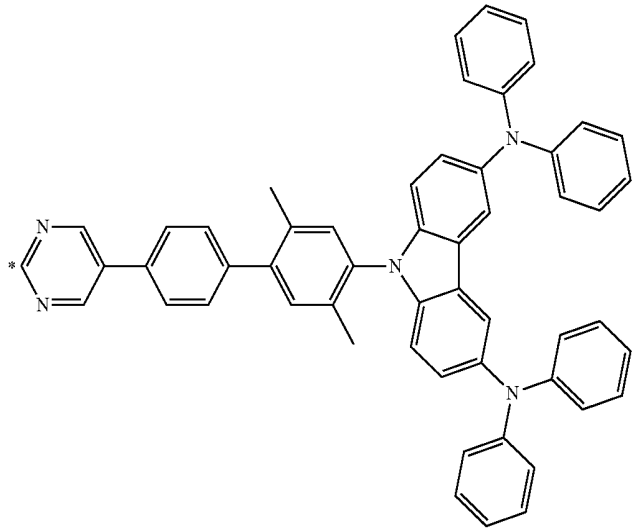
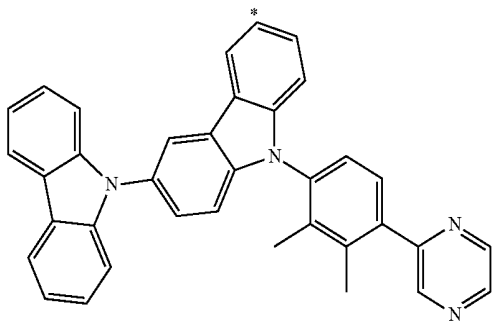


TABLE NN1-continued





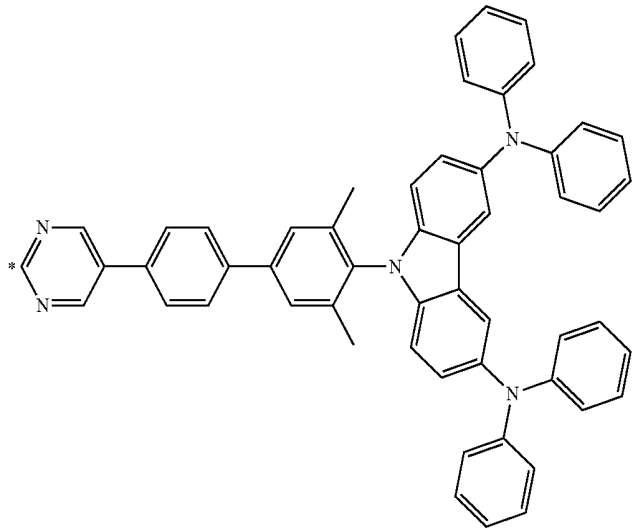
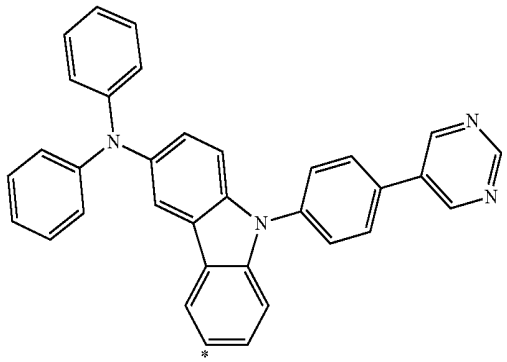
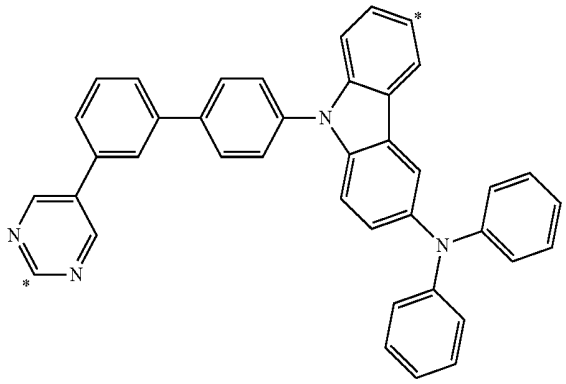
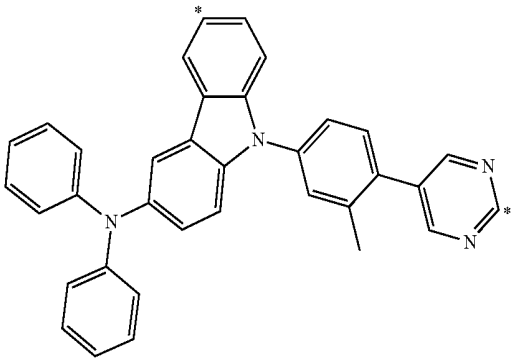
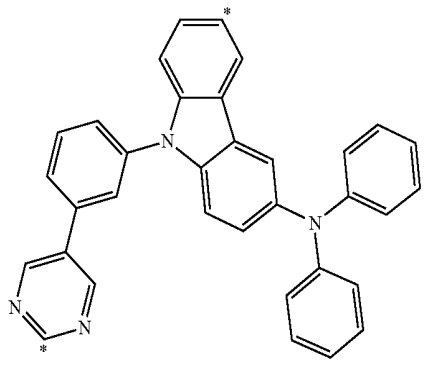


TABLE NN1-continued









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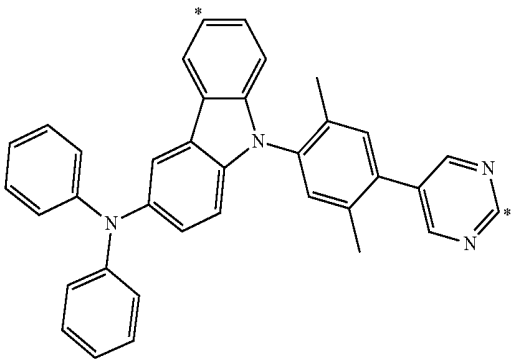
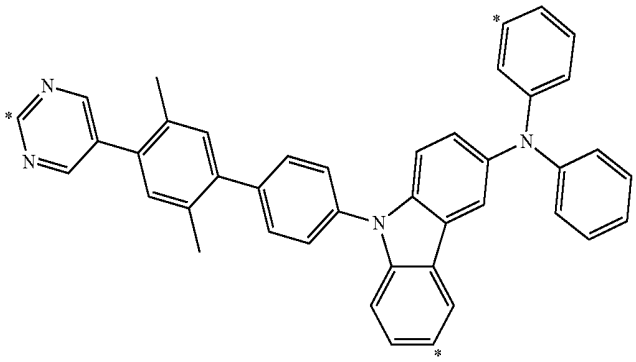
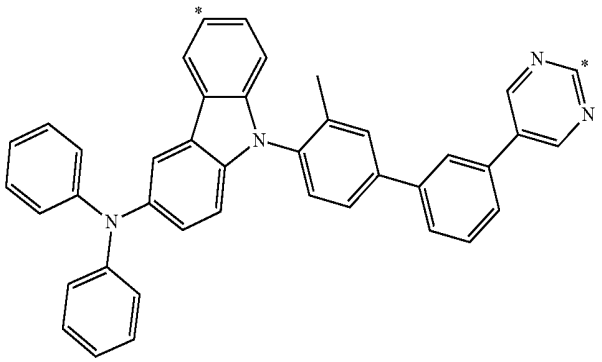






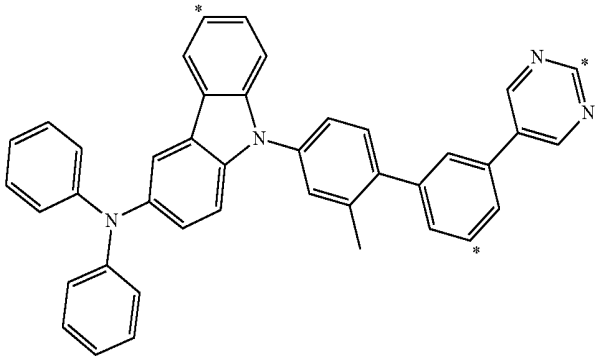
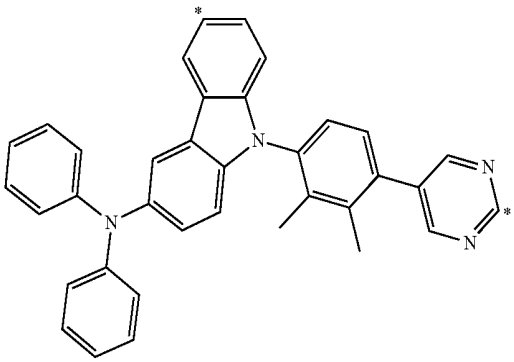
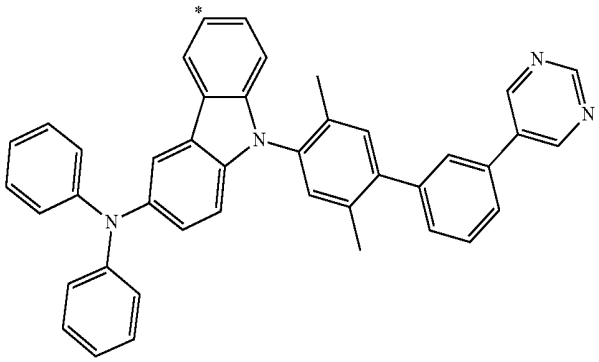


TABLE NN1-continued





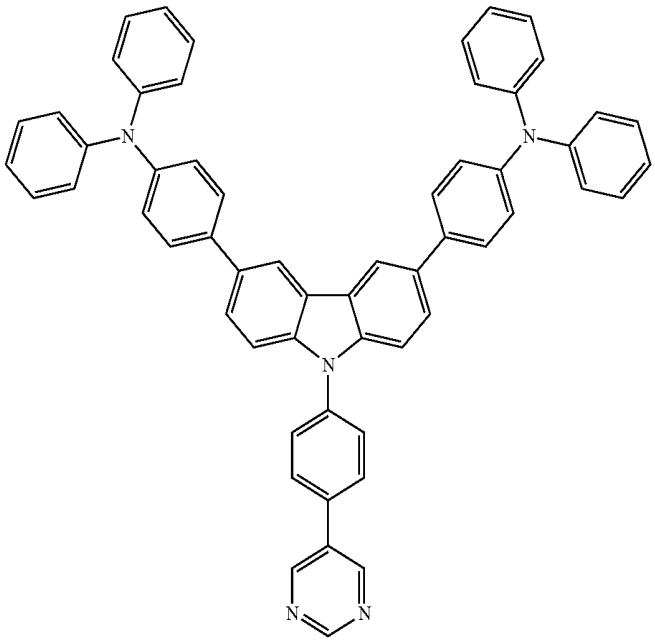
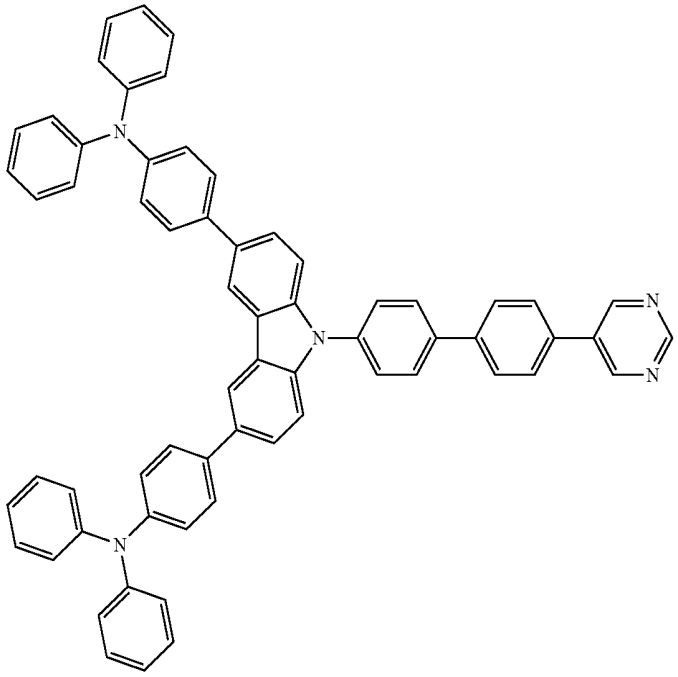
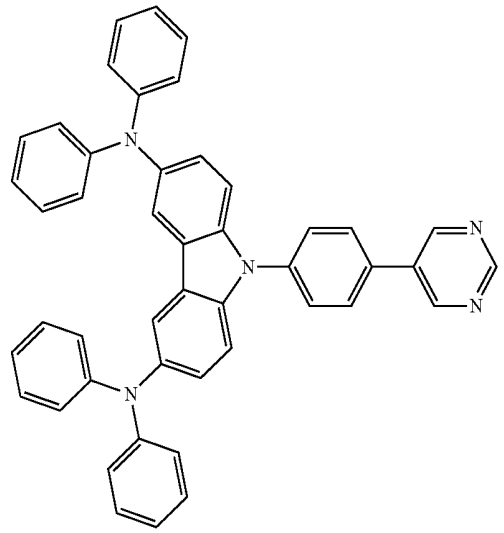


TABLE NN1-continued





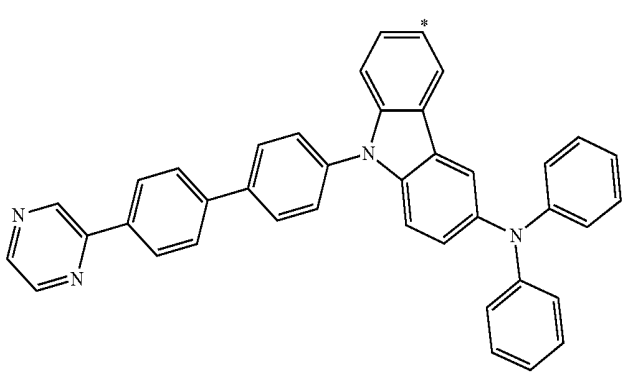
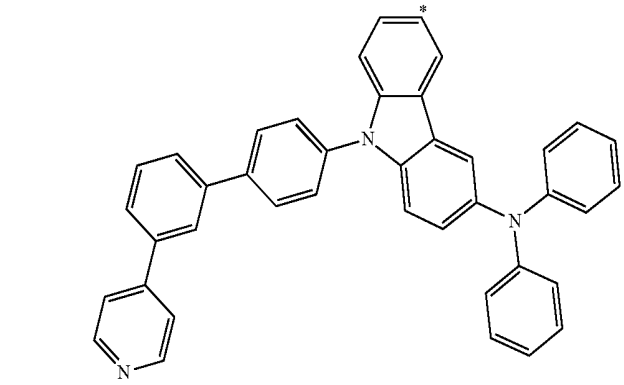
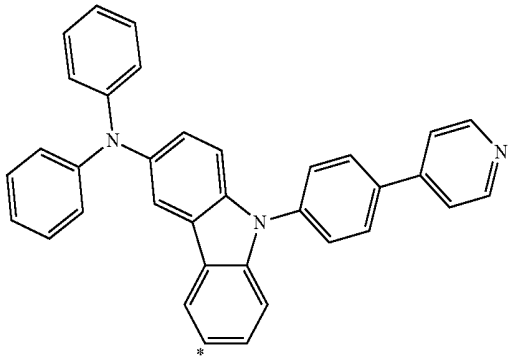
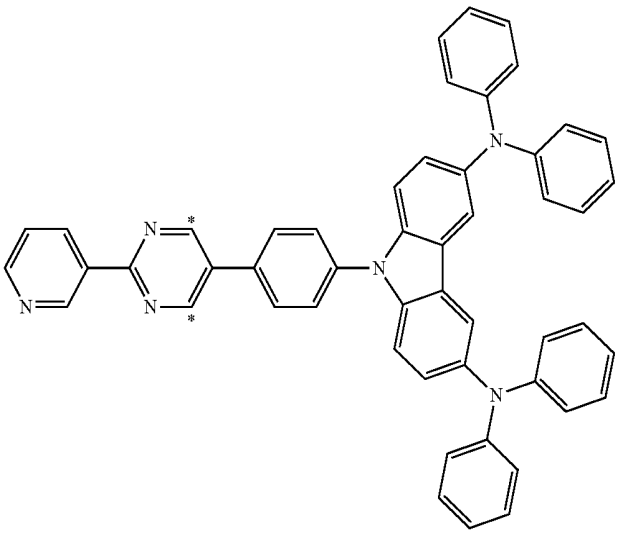


TABLE NN1-continued







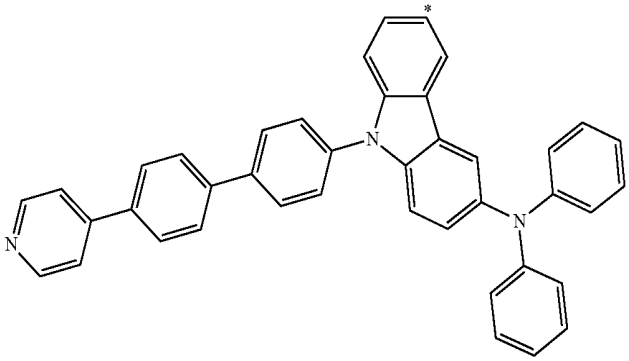
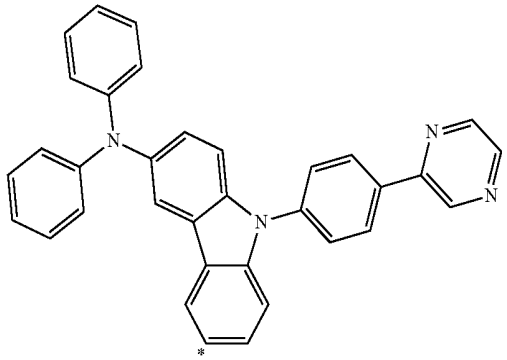
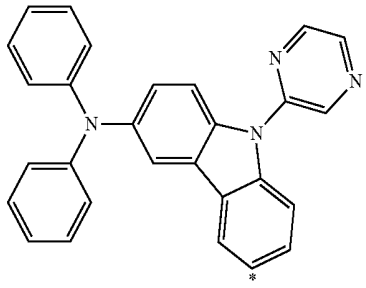
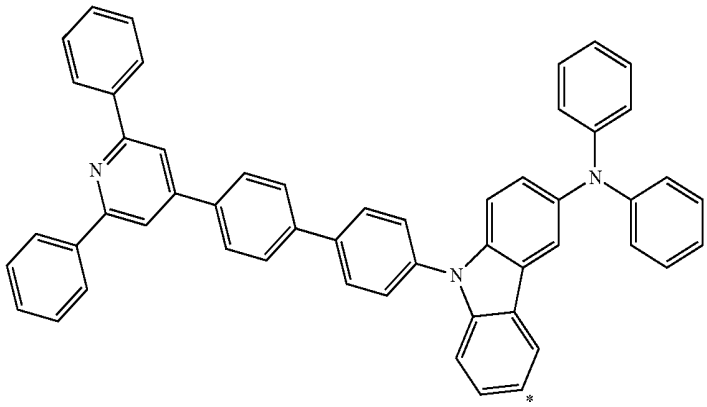


TABLE NN1-continued







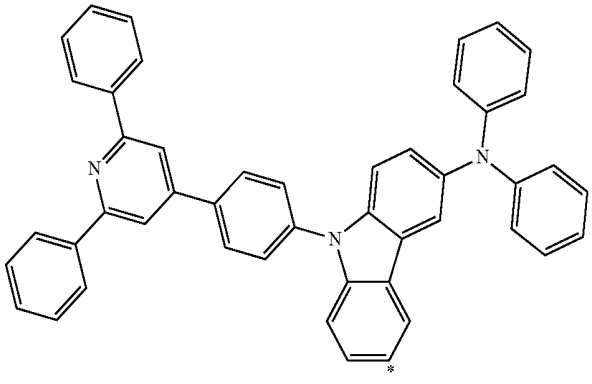
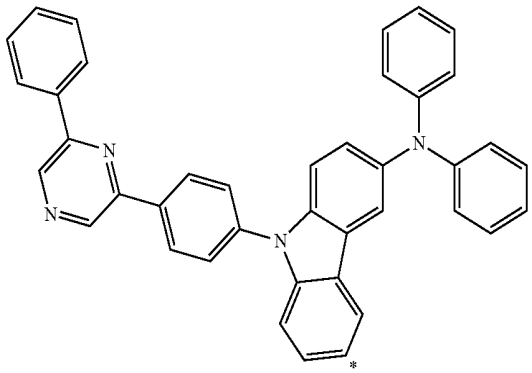
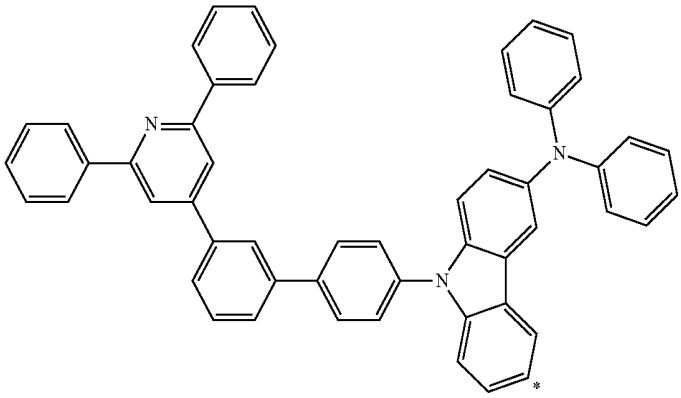


TABLE NN1-continued





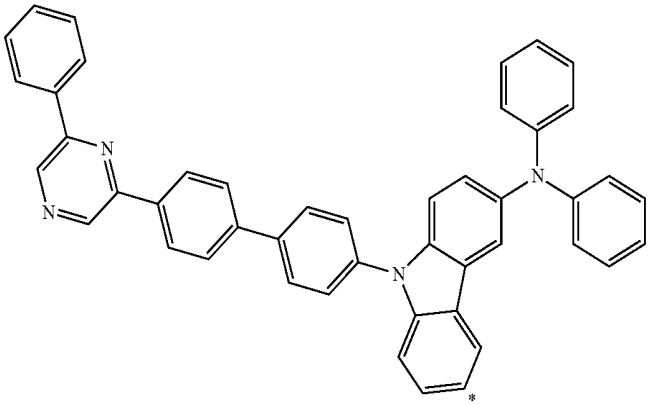
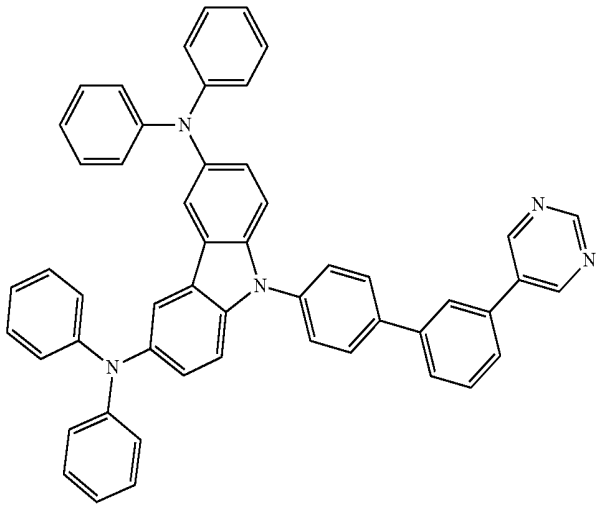
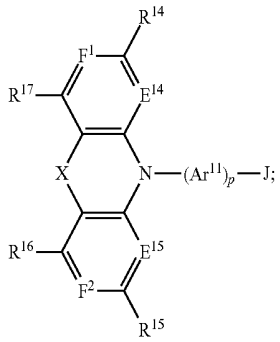


TABLE NN1-continued



[0249] In a sixteenth aspect, the present invention is a compound represented by structural formula (II):

(II)



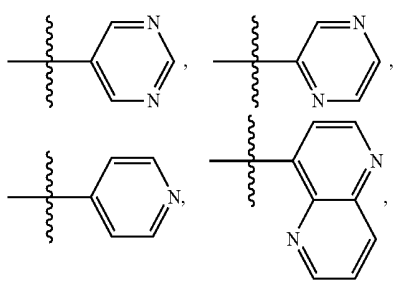
wherein:

[0250] X is O, S, or $C(R^D)_2$;

[0251] R^D, independently for each occurrence, is a C_1-C_6 alkyl or a C_3-C_{18} cycloalkyl;

[0252] E^{14}, and E^{15}, are, each independently, CR^A or N, wherein R^A, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0253] J is any moiety selected from H,



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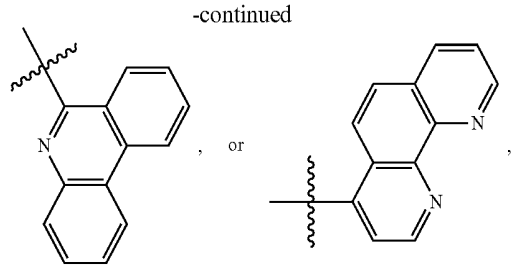


and is optionally substituted with one or more R", each independently selected from is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0254] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0255] F^1 is $C—(Ar^{12})_q$-G;

[0256] F^2 is CR^B or N, wherein R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{18}aryl, a 5-20 atom heteroaryl, a halo, or —CN, or $—(Ar^{12})_q$-G;

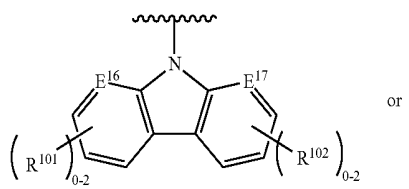
[0257] Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0258] Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0259] p is 0, 1, or 2;

[0260] q is 0 or 1; and

[0261] G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



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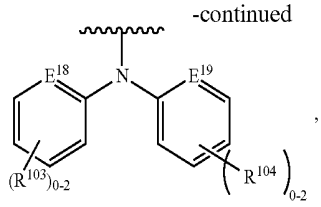


wherein:

[0262] E^{16}, E^{17}, E^{18}, and B^{19} are, each independently, CR^C or N, wherein R^C is H, a C_1-C_3 alkyl, halo, or —CN; and

[0263] R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

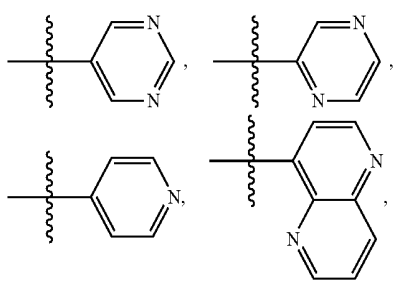
[0264] In certain embodiments of the sixteenth aspect, if $(Ar^{11})_p$-J is phenyl, then F^1 and F^2 are other than CH. In certain embodiments of the fifteenth aspect, the present invention is not represented by any of the compounds in Table NN2. In certain embodiments of the fifteenth aspect, the molecule is not represented by any molecule represented by a structural formula in Table NN2, wherein the carbon or heteroatom denoted by (*) is unsubstituted or substituted by a C_1-C_6 alkyl, —OH , —CN, a halo, a C_6-C_12 aryl, a 5-20 atom heteroaryl, —$N(R^{19})_2$, or —$N(R^{20})_2$, wherein each R^{19}, independently, is H or a C_1-C_6 alkyl, or a C_5-C_{12} cycloalkyl, and wherein each R^{20}, independently, is H or a C_6-C_{18} aryl.

[0265] In certain embodiments of the sixteenth aspect, X is O, S, or $C(R^D)_2$. In certain embodiments, X is O. In certain embodiments, X is S. In certain embodiments, X is $C(R^D)_2$. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0266] In certain embodiments of the sixteenth aspect, R^D, independently for each occurrence, is a C_1-C_6 alkyl or a C_3-C_{18} cycloalkyl. In certain embodiments, R^D, independently for each occurrence, is a C_1-C_3 alkyl. In certain embodiments, R^D, for each occurrence, is methyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0267] In certain embodiments of the sixteenth aspect, E^{14}, and E^{15} are, each independently, CR^A or N. In certain embodiments, E^{14} is CR^A. In certain embodiments, E^{14} is N. In certain embodiments, E^{15} is CR^A. In certain embodiments, E^{15} is N. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0268] In certain embodiments of the sixteenth aspect, J is any moiety selected from —CN,



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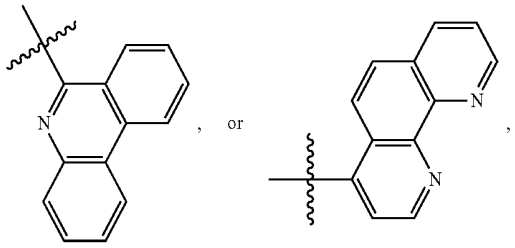
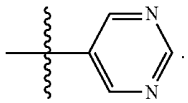
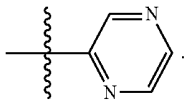


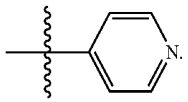
and is optionally substituted with one or more R^{11}. In certain embodiments, J is unsubstituted. In certain embodiments, J is —CN. In certain embodiments, J is



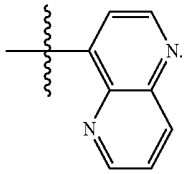
In certain embodiments, J is —CN. In certain embodiments, J is



In certain embodiments, J is —CN. In certain embodiments, J is

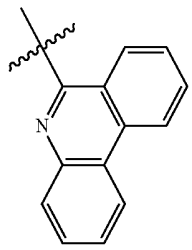


In certain embodiments, J is

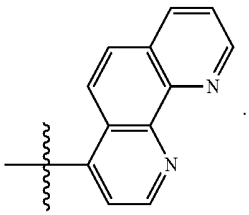


In

[0269] certain embodiments, J is



In certain embodiments, J is



The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0270] In certain embodiments of the sixteenth aspect, each R^{11} is independently selected from C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each is independently selected from C_1-C_6 alkyl or C_6-C_{18} aryl. In certain embodiments, each is independently selected from C_1-C_6 alkyl or phenyl. In certain embodiments, each R^{11} is independently selected from C_1-C_3 alkyl or phenyl. In certain embodiments, each R^{11} is independently selected from methyl or phenyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0271] In certain embodiments of the sixteenth aspect, R^{14} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{14} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{14} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{14} is H or methyl. In certain embodiments, R^{14} is H. In certain embodiments, R^{14} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{14} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{14} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{14} is methyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0272] In certain embodiments of the sixteenth aspect, R^{15} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{15} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{15} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{15} is H or methyl. In certain embodiments, R^{15} is H. In certain embodiments, R^{15} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{15} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{15} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{15} is methyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

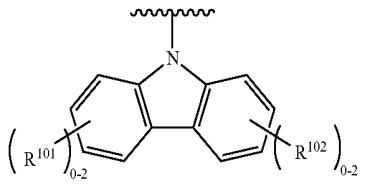
[0273] In certain embodiments of the sixteenth aspect, R^{16} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{16} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{16} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{16} is H or methyl. In certain embodiments, R^{16} is H. In certain embodiments, R^{16} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{16} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{16} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{16} is methyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0274] In certain embodiments of the sixteenth aspect, R^{17} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{17} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{17} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{16} is H or methyl. In certain embodiments, R^{17} is H. In certain embodiments, R^{17} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, R^{17} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, R^{17} is a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{17} is methyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

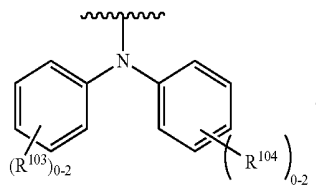
[0275] In certain embodiments of the sixteenth aspect, F^1 is C—$(Ar^{12})_q$-G. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0276] In certain embodiments of the sixteenth aspect, F^2 is N or CR^B. In certain embodiments, F^2 is CR^B. In certain embodiments, F^2 is N. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0277] In certain embodiments of the sixteenth aspect, each R^B is, independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN, or —$(Ar^{12})_q$-G. In certain embodiments, each R^B is, independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or —$(Ar^{12})_q$-G. In certain embodiments, each R^B is, independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or a moiety represented by one of the following structural formulas:

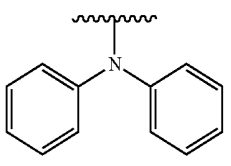


, or



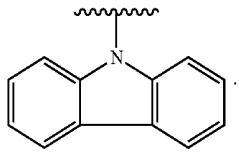
.

In certain embodiments, each R^B is, independently, H or a moiety represented by the following structural formula:

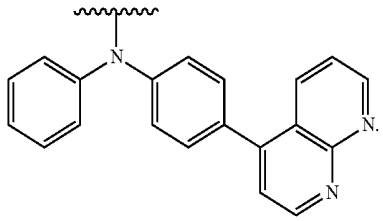


.

In certain embodiments, each R^B is, independently, H or a moiety represented by the following structural formula:



In certain embodiments, each R^B is, independently, H or a moiety represented by the following structural formula:



The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

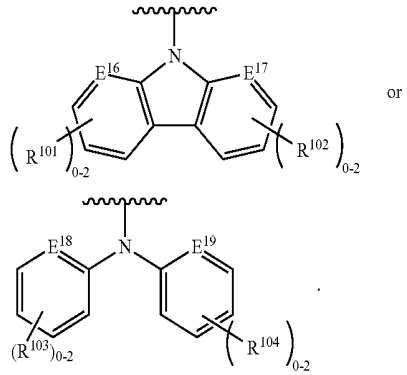
[0278] In certain embodiments of the sixteenth aspect, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four methyls. In certain embodiments, Ar^{11}, for each occurrence, is unsubstituted phenyl. In certain embodiments, Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_2-C_6 alkyls. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0279] In certain embodiments of the sixteenth aspect, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four methyls. In certain embodiments, Ar^{12}, for each occurrence, is unsubstituted phenyl. In certain embodiments, Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_2-C_6 alkyls. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0280] In certain embodiments of the sixteenth aspect, p is 0, 1, or 2. In certain embodiments, p is 0. In certain embodiments, p is 1. In certain embodiments, p is 2. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

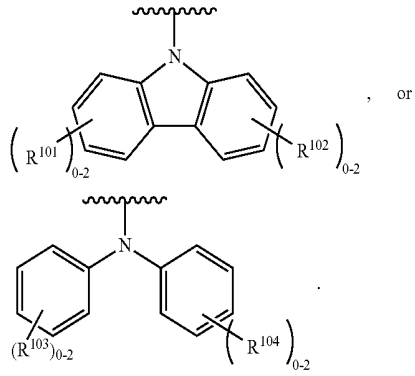
[0281] In certain embodiments of the sixteenth aspect, q is 0 or 1. In certain embodiments, q is 0. In certain embodiments, q is 1. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0282] In certain embodiments of the sixteenth aspect, G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



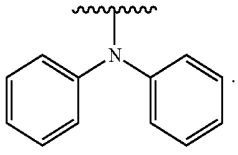
or

In certain embodiments, G is a moiety represented by one of the following structural formulas:

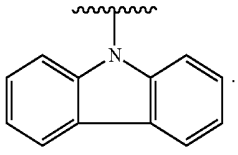


, or

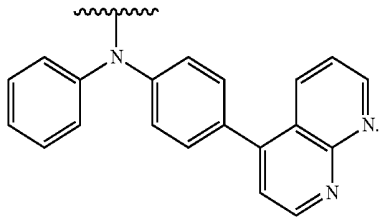
In certain embodiments, G is a moiety represented the following structural formula:



In certain embodiments, G is a moiety represented the following structural formula:



In certain embodiments, G is a moiety represented the following structural formula:



The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0283] In certain embodiments of the sixteenth aspect, E^{16} is CR^C or N. In certain embodiments, E^{16} is CR^C. In certain embodiments, E^{16} is N. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0284] In certain embodiments of the sixteenth aspect, E^{17} is CR^C or N. In certain embodiments, E^{17} is CR^C. In certain embodiments, E^{17} is N. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0285] In certain embodiments of the sixteenth aspect, E^{18} is CR^C or N. In certain embodiments, E^{18} is CR^C. In certain embodiments, E^{18} is N. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0286] In certain embodiments of the sixteenth aspect, E^{19} is CR^C or N. In certain embodiments, E^{19} is CR^C. In certain embodiments, E^{19} is N. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0287] In certain embodiments of the sixteenth aspect, each R^C is, independently, H, a C_1-C_3 alkyl, halo, or —CN. In certain embodiments, each R^C is H. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0288] In certain embodiments of the sixteenth aspect, each R^{102} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each R^{102} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0289] In certain embodiments of the sixteenth aspect, each R^{102} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each R^{102} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0290] In certain embodiments of the sixteenth aspect, each R^{103} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each R^{103} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0291] In certain embodiments of the sixteenth aspect, each R^{104} is, independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each R^{104} is, independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl. The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

[0292] In certain embodiments of the sixteenth aspect:

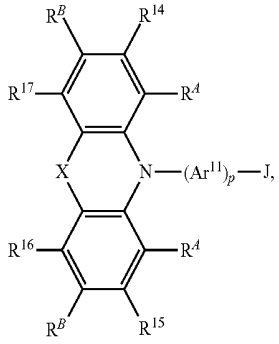
[0293] R^A, for each occurrence independently, is H or a C_1-C_6 alkyl;

[0294] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl; F^2 is CR^B; and

[0295] R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or $—(Ar^{12})_q$-G.

The remainder of the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect.

In certain embodiments of the sixteenth aspect, the molecule is represented by the following structural formula:



wherein the variables in structural formula (II) are as described above and below with respect to the sixteenth aspect. In certain embodiments:

[0296] R^A, for each occurrence independently, is H or a C_1-C_6 alkyl;

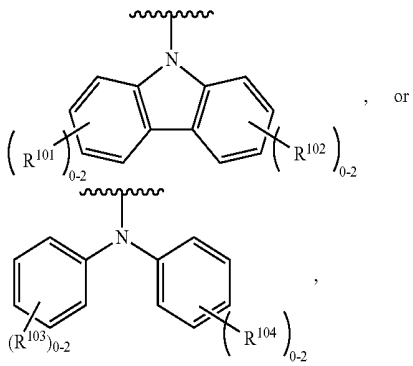
[0297] R^D, for each occurrence, is methyl;

[0298] p is 0 or 1;

[0299] R^{11} is a C_6-C_{18} aryl or a 5-20 atom heteroaryl;

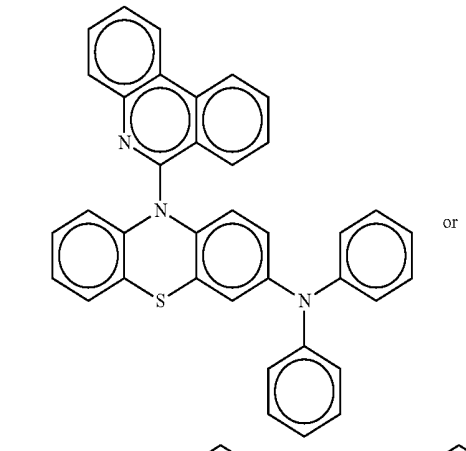
[0300] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN;

[0301] R^B is, for each occurrence independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or a moiety represented by one of the following structural formulas:



[0302] R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl, a C_3-C_{10} cycloalkyl, a C_6-C_{10} aryl, or a 5-10 atom heteroaryl.

[0303] In certain embodiments of the sixteenth aspect, the molecule is represented by one of the following structural formulas:



or

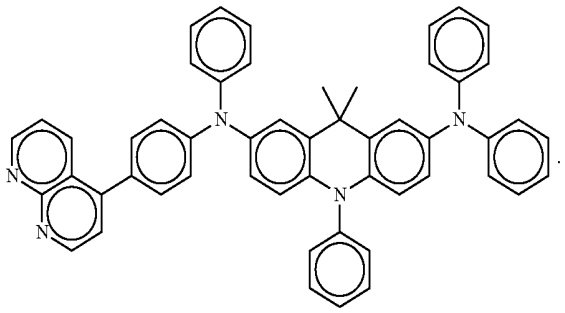
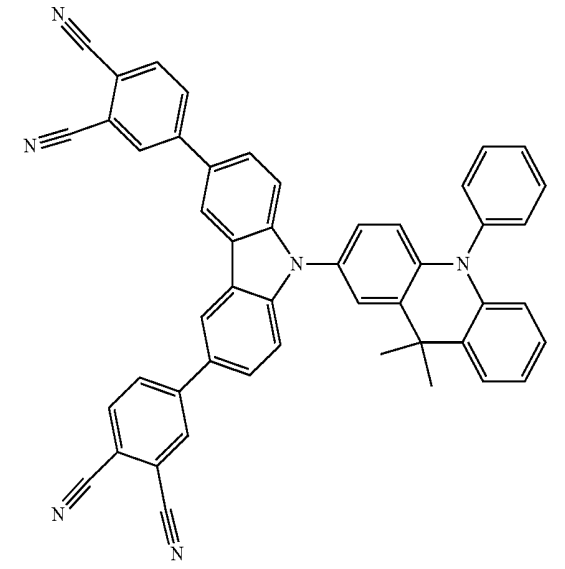


TABLE NN2



[0304] In a seventeenth aspect, the present invention is a compound represented by one of structural formulas (IIIA), (IIIB), (IIIC), (IIID), or (IIIE):

PA (IIIA)

PAP (IIIB)

PPA (IIIC)

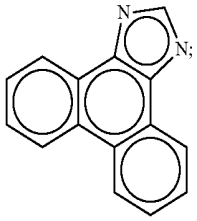
PAA (IIID)

APA (IIIE)

In structural formulas (IIIA)-(IIIE):

[0305] The moieties P and A are either covalently linked or are linked by a moiety φ;

[0306] P is represented by the following structural formula:



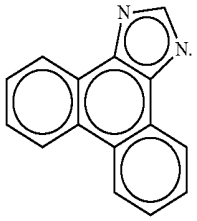
[0307] each instance of P, independently, is optionally substituted with one or more groups R^{31}, each independently selected from a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

[0308] each instance of P is, independently, linked to the remainder of the molecule by any one atom in the heterocyclic ring portion;

[0309] each instance of φ, independently, phenyl optionally substituted with one to four C_1-C_6 alkyls; and

[0310] A is a 5-20 atom heteroaryl, optionally substituted with one or more groups R^{32}, each independently selected from a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0311] In certain embodiments of the seventeenth aspect, P is represented by the following structural formula:



In certain embodiments, each instance of P, independently, is optionally substituted with one or more R^{31}. In certain embodiments, each instance of P is unsubstituted. The remainder of the variables in structural formulas (IIIA)-(IIIE)are as defined above and below with respect to the seventeenth aspect.

[0312] In certain embodiments of the seventeenth aspect, each instance of φ, independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, each instance of φ, independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, each instance of φ, independently, is phenyl optionally substituted with one to four methyls. In certain embodiments, each instance of φ, independently, is unsubstituted phenyl. The remainder of the variables in structural formulas (IIIA)-(IIIE) are as defined above and below with respect to the seventeenth aspect.

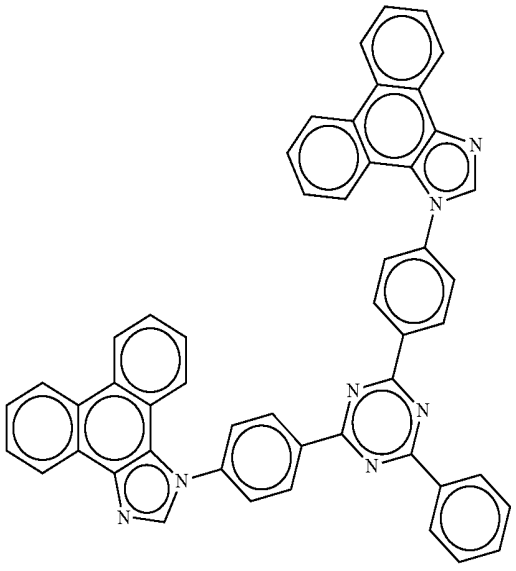
[0313] In certain embodiments of the seventeenth aspect, each instance of A, independently, is a 5-20 atom heteroaryl,

optionally substituted with one or more R^{32}. In certain embodiments, each instance of A, independently, is pyridinyl, pyrimidinyl, triazinyl, quinoline, isoquinoline, or a diazanaphthalene. In certain embodiments, each instance of A, independently, is triazinyl or 1,4-diazanaphthalene. In certain embodiments, each instance of A, independently, is 1,4-diazanaphthalene. In certain embodiments, each instance of A, independently, is triazinyl. In certain embodiments, each instance of A, independently, is unsubstituted. The remainder of the variables in structural formulas (IIIA)-(IIIE)are as defined above and below with respect to the seventeenth aspect.

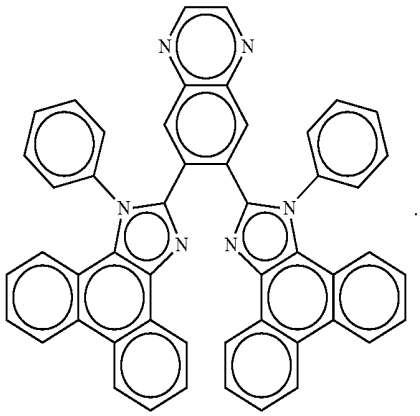
[0314] In certain embodiments of the seventeenth aspect, each instance of R^{31} is independently selected from φ, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each instance of R^{31} is independently selected from φ, C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, each instance of R^{31} is independently selected from φ or methyl. In certain embodiments, each instance of R^{31} is independently selected from φ. The remainder of the variables in structural formulas (IIIA)-(IIIE)are as defined above and below with respect to the seventeenth aspect.

[0315] In certain embodiments of the seventeenth aspect, each instance of R^{32} is independently selected from φ, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. In certain embodiments, each instance of R^{32} is independently selected from φ, C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN. In certain embodiments, each instance of R^{32} is independently selected from φ or methyl. In certain embodiments, each instance of R^{32} is independently selected from φ. The remainder of the variables in structural formulas (IIIA)-(IIIE) are as defined above and below with respect to the seventeenth aspect.

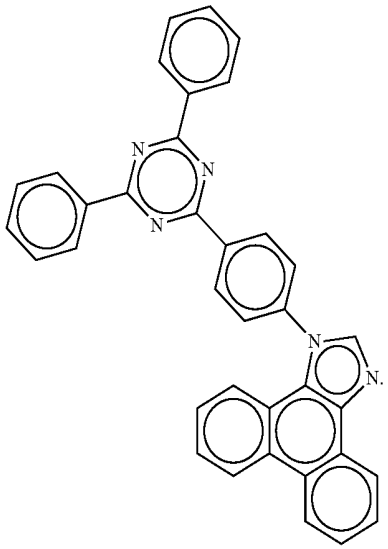
[0316] In certain embodiments of the seventeenth aspect, the molecule is represented by structural formula (IIIA). The variables are as defined above with respect to the seventeenth aspect. In certain embodiments, the molecule is represented by the following structural formula:



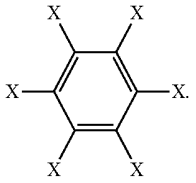
[0317] In certain embodiments of the seventeenth aspect, the molecule is represented by structural formula (IIIB). The variables are as defined above with respect to the seventeenth aspect. In certain embodiments, the molecule is represented by the following structural formula:



[0318] In certain embodiments of the seventeenth aspect, the molecule is represented by structural formula (IIIC). The variables are as defined above with respect to the seventeenth aspect. In certain embodiments, the molecule is represented by the following structural formula:



[0319] In an eighteenth aspect, the present invention is a compound represented by structural formula (IV):



(IV)

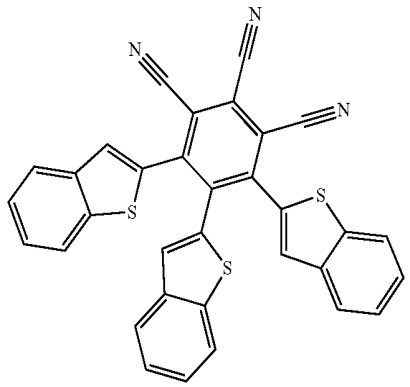
In structural formula (IV):

[0320] each X is, independently, selected from H, C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or $—(Ar^{21})_d$-G;

[0321] d, for each occurrence independently, is 0, 1, or 2;

[0322] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0323] G, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments, at least one instance of X is $—(Ar^{21})_d$-G^4, wherein G^4 is benzothiophene. In certain embodiments, at least one instance of X is —CN. In certain embodiments, the molecule is not represented by the following structural formula:

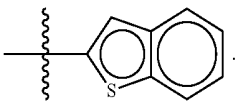


[0324] In certain embodiments of the eighteenth aspect, each X is, independently, selected from H, C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or $—(Ar^{21})_d$-G. In certain embodiments, each X is, independently, selected from C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or $—(Ar^{21})_d$-G. In certain embodiments, each X is, independently, selected from H, —CN, or $—(Ar^{21})_d$-G. In certain embodiments, at least two instances of X are $—(Ar^{21})_d$-G^4. In certain embodiments, at least three instances of X are $—(Ar^{21})_d$-G^4. In certain embodiments, at least four instances of X are $—(Ar^{21})_d$-G^4. In certain embodiments, at least two instances of X are —CN. In certain embodiments, at least three instances of X are —CN. In certain embodiments, at least four instances of X are —CN. In certain embodiments, three instances of X are $—(Ar^{21})_d$-G^4 and three instances of X are —CN. The remainder of the variables in structural formula (IV) are as defined above and below with respect to the eighteenth aspect.

[0325] In certain embodiments of the eighteenth aspect, d, for each occurrence independently, is 0, 1, or 2. In certain embodiments, d, for each occurrence independently, is 0 or 1. In certain embodiments, d, for each occurrence independently, is 0. In certain embodiments, d, for each occurrence independently, is 1. In certain embodiments, d, for each occurrence independently, is 2. The remainder of the variables in structural formula (IV) are as defined above and below with respect to the eighteenth aspect.

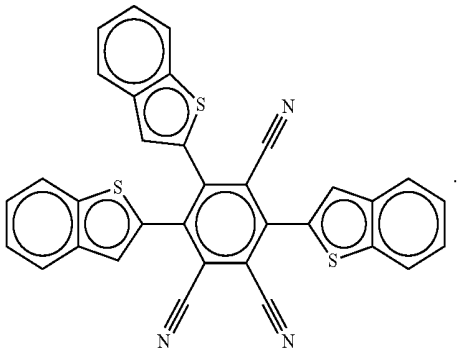
[0326] In certain embodiments of the eighteenth aspect, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four methyls. In certain embodiments, Ar^{21}, for each occurrence, is unsubstituted phenyl. In certain embodiments, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_2-C_6 alkyls. The remainder of the variables in structural formula (IV) are as defined above and below with respect to the eighteenth aspect.

[0327] In certain embodiments of the eighteenth aspect, G, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments, G is benzothiophene. In certain embodiments, G is represented by the following structural formula:



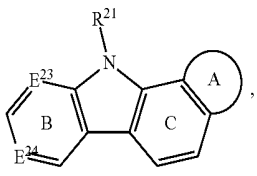
The remainder of the variables in structural formula (IV) are as defined above and below with respect to the eighteenth aspect.

[0328] In certain embodiments of the eighteenth aspect, the molecule is represented by the following structural formula:

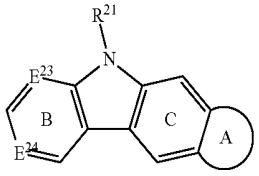


[0329] In a nineteenth aspect, the present invention is a compound represented by structural formula (VA), (VB), or (VC):

(VA)



(VB)



or

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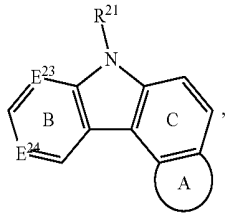
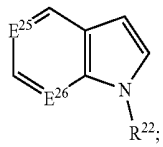
(VC)



According to structural formulas (VA), (VB), and (VC):

[0330] Ring A, for each occurrence independently, is represented by the following structural formula:

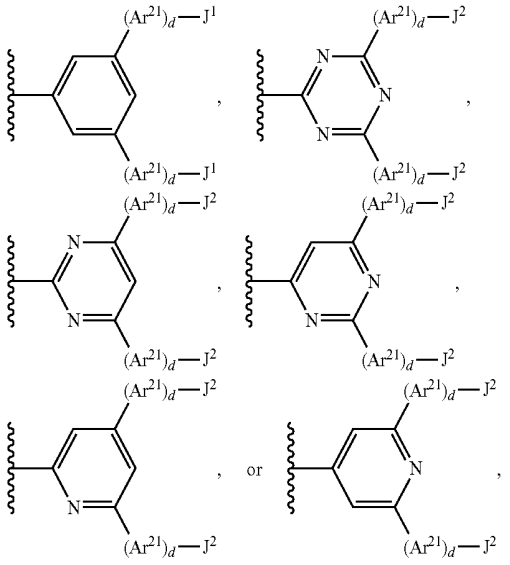


[0331] Rings A, B, and C, each independently, are optionally substituted with 1 or 2 substituents selected from a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN;

[0332] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, —$(Ar^{21})_d$-G, or —Ar^{22}, provided that at least one of R^{21} and R^{22} is —$(Ar^{21})_d$-G or —$(Ar^{21})_d$—Ar^{22};

[0333] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

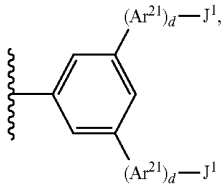
[0334] Ar^{22}, for each occurrence independently, is:



[0335] and is optionally substituted with one to three C_1-C_6 alkyls;

[0336] d, for each occurrence independently, is 0, 1, or 2;

[0337] J^1, for each occurrence independently, is H, C_6-C_{18} aryl or 5-20 atom heteroaryl and is optionally substituted by one or more —CN, —C(O)phenyl, C_1-C_6 alkyl, C_1-C_6 haloalkyl, C_6-C_{18} aryl, or (5-6 atom) heteroaryl, provided that if at least one instance of Ar^{22} is



then at least one J^1 is not H or unsubstituted phenyl;

[0338] J^2, for each occurrence independently, is H, C_6-C_{18} aryl or 5-20 atom heteroaryl and is optionally substituted by one or more —CN, —C(O)phenyl, C_1-C_6 alkyl, C_1-C_6 haloalkyl, C_6-C_{18} aryl, or (5-6 atom) heteroaryl;

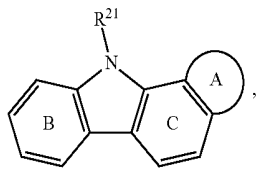
[0339] G, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl, provided that G is not triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl, further provided that if G is phenyl it is not unsubstituted and is not substituted with carbonyl, trifluoromethyl, triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl; and

[0340] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

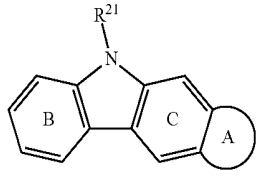
[0341] In certain embodiments of the nineteenth aspect, the compound is not represented by any structural formula in Table NR. In certain embodiments of the fifteenth aspect, the molecule is not represented by any molecule represented by a structural formula in Table NR, wherein the carbon or heteroatom denoted by (*) is unsubstituted or substituted by a C_1-C_6 alkyl, —OH , —CN, a halo, a C_6-C_12 aryl, a 5-20 atom heteroaryl, —$N(R^{19})_2$, or —$N(R^{20})_2$, wherein each R^{19}, independently, is H or a C_1-C_6 alkyl, or a C_5-C_{12} cycloalkyl, and wherein each R^{20}, independently, is H or a C_6-C_{18} aryl.

[0342] In certain embodiments of the nineteenth aspect, the molecule is represented by any one of structural formulas (VD), (VE), or (VF):

(VD)



(VE)



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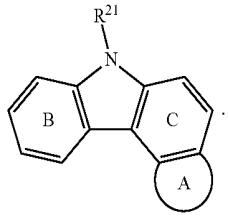
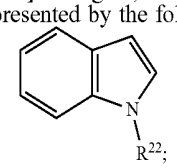
(VF)



In structural formulas (VD), (VE), and (VF):

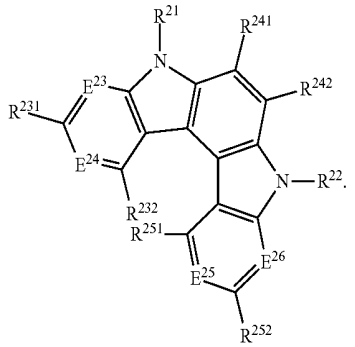
[0343] Ring A, for each occurrence independently, is represented by the following structural formula:



and rings A, B, and C, each independently, are optionally substituted with 1 to 4 substituents selected from a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. The remainder of the variables in structural formulas (VD), (VE), and (VF) are as defined above and below with respect to the nineteenth aspect.

[0344] In certain embodiments of the nineteenth aspect, the molecule is represented by structural formula (VG):

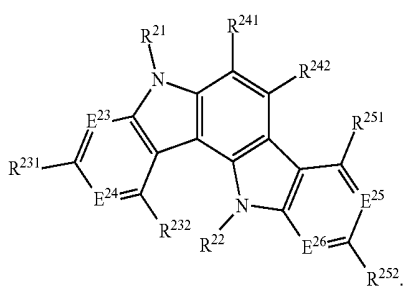
(VG)



In structural formula (VG), R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. The remainder of the variables in structural formula (VG) are as defined above and below with respect to the nineteenth aspect.

[0345] In certain embodiments of the nineteenth aspect, the molecule is represented by structural formula (VH):

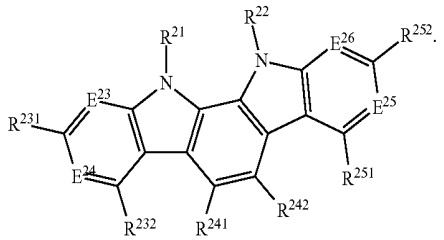
(VH)



In structural formula (VH), R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. The remainder of the variables in structural formula (VH) are as defined above and below with respect to the nineteenth aspect.

[0346] In certain embodiments of the nineteenth aspect, the molecule is represented by structural formula (VJ):

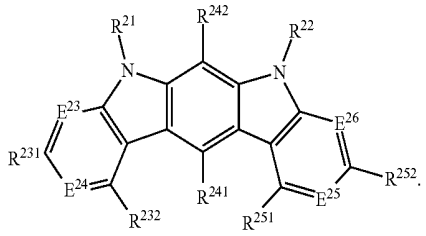
(VJ)



In structural formula (VJ), R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. The remainder of the variables in structural formula (VJ) are as defined above and below with respect to the nineteenth aspect.

[0347] In certain embodiments of the nineteenth aspect, the molecule is represented by structural formula (VK):

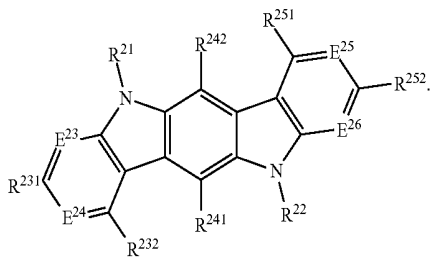
(VK)



In structural formula (VK), R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. The remainder of the variables in structural formula (VK) are as defined above and below with respect to the nineteenth aspect.

[0348] In certain embodiments of the nineteenth aspect, the molecule is represented by structural formula (VL):

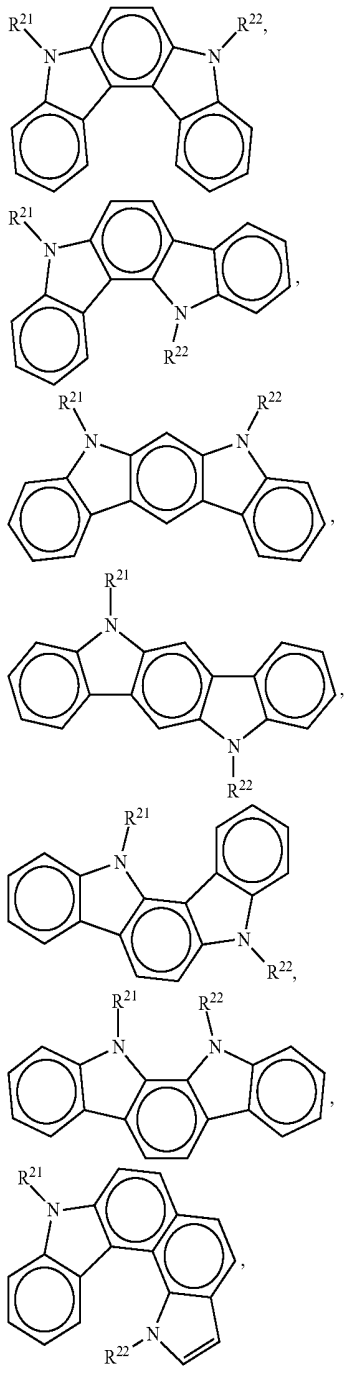
(VL)



In structural formula (VL), R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18}

cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. The remainder of the variables in structural formula (VL) are as defined above and below with respect to the nineteenth aspect.

[0349] In certain embodiments of the nineteenth aspect, ring A may be fused to ring C in any orientation. In certain embodiments, any two atoms of the six-membered ring in ring A may be shared with ring C. In other embodiments, the two carbon atoms of the five-membered ring ing ring A may be shared with ring C. In example embodiments, the compounds of structures (VA), (VB), and (VC) can be represented by the following structural formulas:



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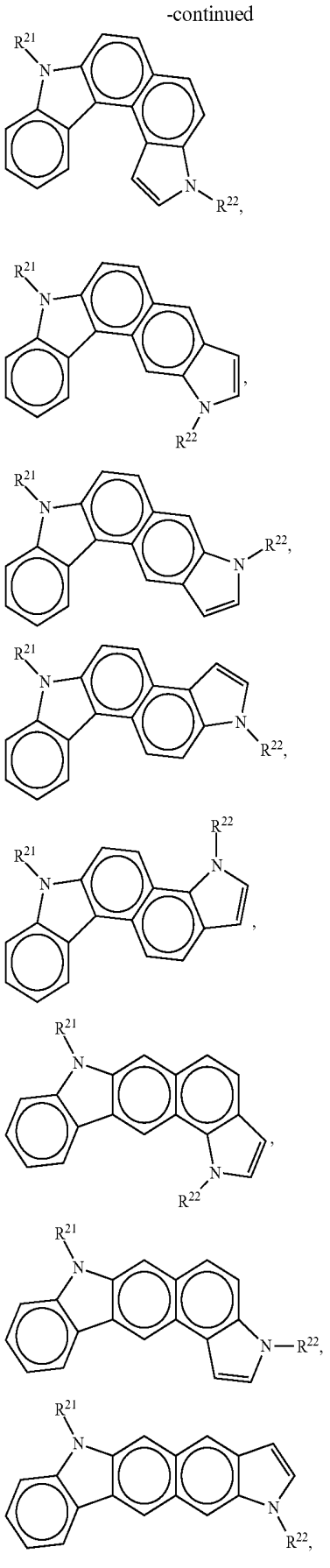

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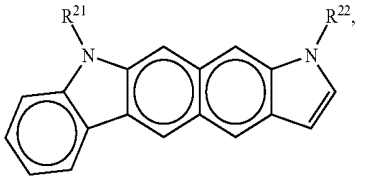

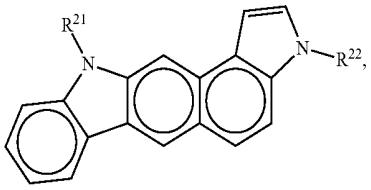

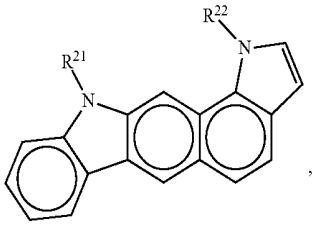

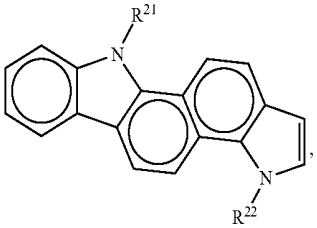

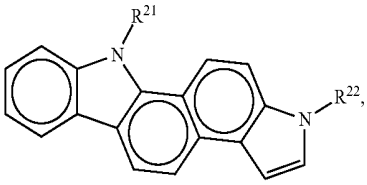

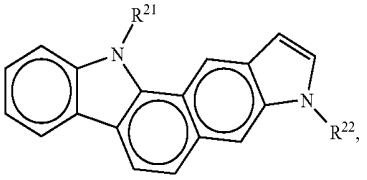

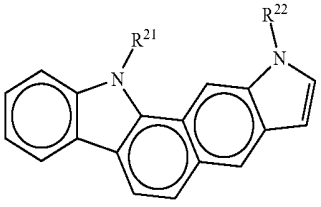

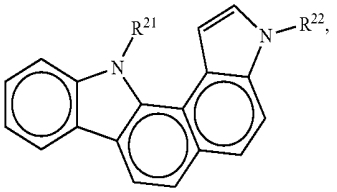

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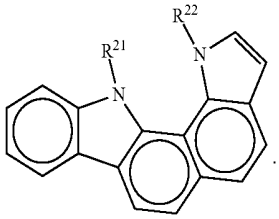


The remainder of the variables in structural formulas (VA)-(VL) are as defined above and below with respect to the nineteenth aspect.

[0350] In certain embodiments of the nineteenth aspect, R^{21} is selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, —$(Ar^{21})_d$-G, or —Ar^{22}. According to certain embodiments, R^{21} is selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or —$(Ar^{21})_d$—Ar^{22}. According to certain embodiments, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or —$(Ar^{21})_d$-G. According to certain embodiments, R^{21} is selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, —$(Ar^{21})_d$-G, or —Ar^{22}. According to certain embodiments, R^{21} is selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or —Ar^{22}. According to certain embodiments, R^{21} is selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or —$(Ar^{21})_d$-G. The remainder of the variables in structural formulas (VA)-(VL) are as defined above and below with respect to the nineteenth aspect.

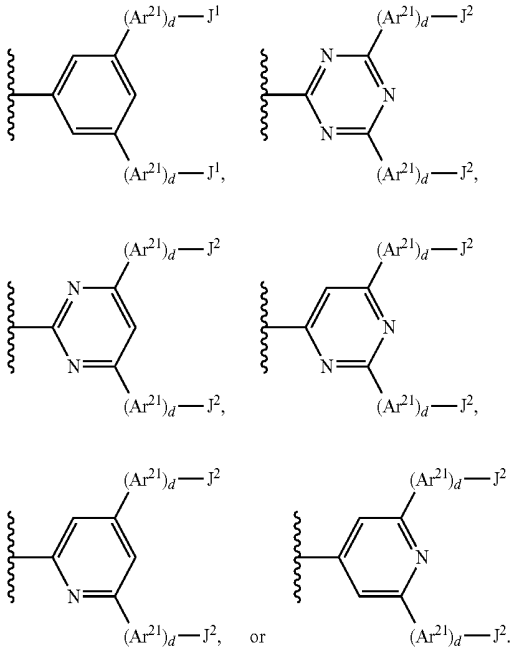
[0351] In certain embodiments of the nineteenth aspect, R^{22} is selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, —$(Ar^{21})_d$-G, or —Ar^{22}. According to certain embodiments, R^{22} is selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or —$(Ar^{21})_d$—Ar^{22}. According to certain embodiments, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or —$(Ar^{21})_d$-G. According to certain embodiments, R^{22} is selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, —$(Ar^{21})_d$-G, or —Ar^{22}. According to certain embodiments, R^{22} is selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or —Ar^{22}. According to certain embodiments, R^{22} is selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or —$(Ar^{21})_d$-G. The remainder of the variables in structural formulas (VA)-(VL) are as defined above and below with respect to the nineteenth aspect.

[0352] According to certain embodiments of the nineteenth aspect, at least one of R^{21} and R^{22} is —$(Ar^{21})_d$-G or —$(Ar^{21})_d$—Ar^{22}. According to certain embodiments, at least one of R^{21} and R^{22} is —$(Ar^{21})_d$-G. According to certain embodiments, at least one of R^{21} and R^{22} is —$(Ar^{21})_d$-Ar^{22}. According to certain embodiments, one of R^{21} and R^{22} is H or unsubstituted phenyl. According to certain embodiments, one of R^{21} and R^{22} is H. According to certain embodiments, one of R^{21} and R^{22} is unsubstituted phenyl. According to certain embodiments, R^{21} and R^{22} are identical.

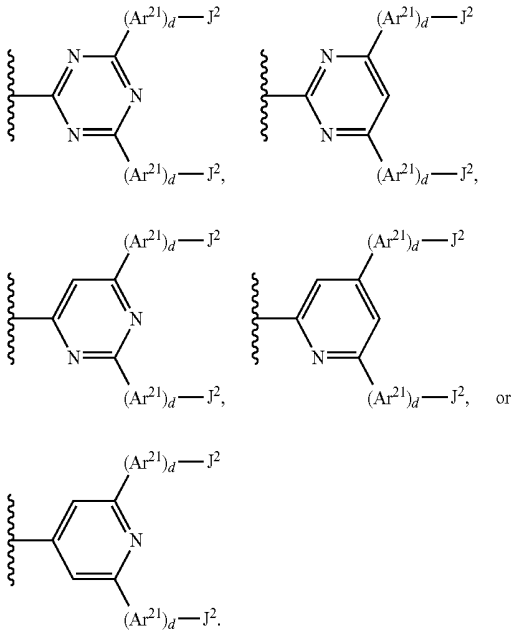
[0353] In certain embodiments of the nineteenth aspect, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four

methyls. In certain embodiments, Ar^{21}, for each occurrence, is unsubstituted phenyl. In certain embodiments, Ar^{21}, for each occurrence independently, is phenyl substituted with one to four C_2-C_6 alkyls. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

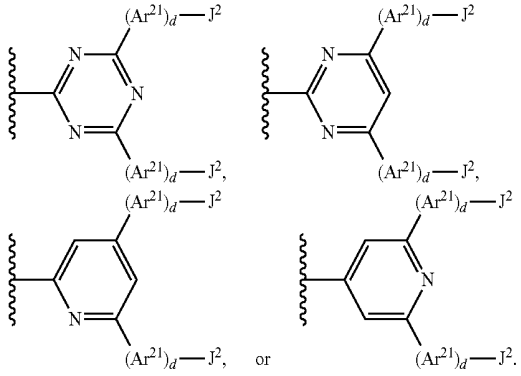
[0354] In certain embodiments of the nineteenth aspect, Ar^{22}, for each occurrence independently, is:



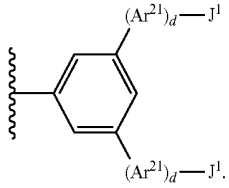
[0355] In certain embodiments, Ar^{22}, for each occurrence independently, is:



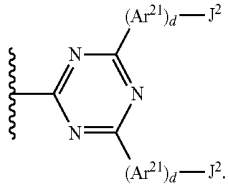
In certain embodiments, Ar^{22}, for each occurrence independently, is:



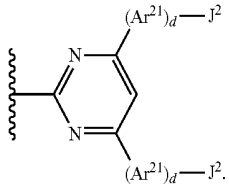
In certain embodiments, Ar^{22}, for each occurrence, is



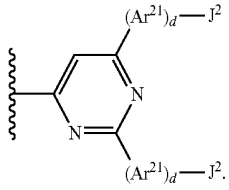
In certain embodiments, Ar^{22}, for each occurrence, is



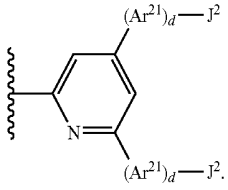
In certain embodiments, Ar^{22}, for each occurrence, is



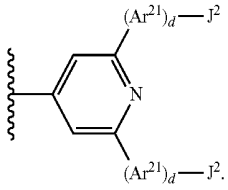
In certain embodiments, Ar^{22}, for each occurrence, is



In certain embodiments, Ar^{22}, for each occurrence, is



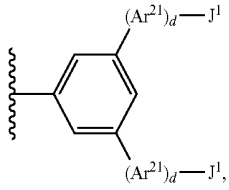
In certain embodiments, Ar^{22}, for each occurrence, is



In certain embodiments, Ar^{22}, for each occurrence independently, is optionally substituted with one to four C_1-C_6 alkyls. In certain embodiments, Ar^{22}, for each occurrence independently, is optionally substituted with one to four C_1-C_3 alkyls. In certain embodiments, Ar^{22}, for each occurrence independently, is optionally substituted with one to four methyls. In certain embodiments, Ar^{22}, for each occurrence, is unsubstituted. In certain embodiments, Ar^{22}, for each occurrence independently, is substituted with one to four C_2-C_6 alkyls. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0356] In certain embodiments of the nineteenth aspect, d, for each occurrence independently, is 0, 1, or 2. In certain embodiments, d, for each occurrence independently, is 0 or 1. In certain embodiments, d is 0. In certain embodiments, d is 1. In certain embodiments, d is 2. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0357] In certain embodiments of the nineteenth aspect, J^1, for each occurrence independently, is H, C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments of the nineteenth aspect, J^1, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments of the nineteenth aspect, J^1, for each occurrence independently, is phenyl or pyridinyl. In certain embodiments of the nineteenth aspect, J^1, for each occurrence, is phenyl. In certain embodiments of the nineteenth aspect, J^1, for each occurrence, is pyridinyl. In certain embodiments, J^1 is optionally substituted with one or more —CN, —C(O)phenyl, C_1-C_6 alkyl, C_1-C_6 haloalkyl, C_6-C_{18} aryl, or (5-6 atom) heteroaryl. In certain embodiments, J^1 is optionally substituted with —CN, C_1-C_3 alkyl, C_1-C_3 haloalkyl, C_6-C_{10} aryl, or (5-6 atom) heteroaryl. In certain embodiments, J^1 is optionally substituted with —CN, or C_1-C_6 haloalkyl. In certain embodiments, J^1 is optionally substituted with phenyl, trifluoromethyl, or cyano. In certain embodiments, J^1 is unsubstituted. In certain embodiments, J^1 is substituted as described herein. In certain embodiments, if at least one instance of Ar^{22} is



then at least one J^1 is not H or unsubstituted phenyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0358] In certain embodiments of the nineteenth aspect, J^2, for each occurrence independently, is H, C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments of the nineteenth aspect, J^2, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments of the nineteenth aspect, J^2, for each occurrence independently, is phenyl or pyridinyl. In certain embodiments of the nineteenth aspect, J^2, for each occurrence, is phenyl. In certain embodiments of the nineteenth aspect, J^2, for each occurrence, is pyridinyl. In certain embodiments, J^2 is optionally substituted with one or more —CN, —C(O)phenyl, C_1-C_6 alkyl, C_1-C_6 haloalkyl, C_6-C_{18} aryl, or (5-6 atom) heteroaryl. In certain embodiments, J^2 is optionally substituted with —CN, C_1-C_3 alkyl, C_1-C_3 haloalkyl, C_6-C_{10} aryl, or (5-6 atom) heteroaryl. In certain embodiments, J^2 is optionally substituted with —CN, or C_1-C_6 haloalkyl. In certain embodiments, J^2 is optionally substituted with phenyl, trifluoromethyl, or cyano. In certain embodiments, J^2 is unsubstituted. In certain embodiments, J^2 is substituted as described herein. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0359] In certain embodiments of the nineteenth aspect, G, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl. In certain embodiments, G is optionally substituted with one or more —CN, —C(O)phenyl, C_1-C_6 alkyl, C_1-C_6 haloalkyl, C_6-C_{18} aryl, or (5-6 atom) heteroaryl. In certain embodiments, G is optionally substituted with —CN, C_1-C_3 alkyl, C_1-C_3 haloalkyl, C_6-C_{10} aryl, or (5-6 atom) heteroaryl. In certain embodiments, G is optionally substituted with —CN, or C_1-C_6 haloalkyl. In certain embodiments, G is optionally substituted with phenyl, trifluoromethyl, or cyano. In certain embodiments, G is unsubstituted. In certain embodiments, G is substituted as described herein. In certain embodiments, G is not triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl. In certain embodiments, if G is phenyl it is not unsubstituted and is not substituted with carbonyl, trifluoromethyl, triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl. In certain embodiments, G is phenyl substituted with up to 5 C_1-C_6 haloalkyls. In certain embodiments, G is phenyl substituted with up to 5 trifluoromethyls. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0360] In certain embodiments of the nineteenth aspect, E^{23} is CR^Y or N. In certain embodiments, E^{23} is N. In certain embodiments, E^{23} is CR^Y. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0361] In certain embodiments of the nineteenth aspect, E^{24} is CR^Y or N. In certain embodiments, E^{24} is N. In certain embodiments, E^{24} is CR^Y. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0362] In certain embodiments of the nineteenth aspect, E^{25} is CR^Y or N. In certain embodiments, E^{25} is N. In certain embodiments, E^{25} is CR^Y. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0363] In certain embodiments of the nineteenth aspect, E^{26} is CR^Y or N. In certain embodiments, E^{26} is N. In certain embodiments, E^{26} is CR^Y. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0364] In certain embodiments of the nineteenth aspect, R^Y, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^Y, for each occurrence independently, is H or a C_1-C_6 alkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0365] In certain embodiments of the nineteenth aspect, R^{231} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^{231} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{231} is H. In certain embodiments, R^{231} is a C_1-C_6 alkyl, phenyl, or a C_3-C_6 cycloalkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0366] In certain embodiments of the nineteenth aspect, R^{232} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^{232} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{232} is H. In certain embodiments, R^{232} is a C_1-C_6 alkyl, phenyl, or a C_3-C_6 cycloalkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0367] In certain embodiments of the nineteenth aspect, R^{241} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^{241} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{241} is H. In certain embodiments, R^{241} is a C_1-C_6 alkyl, phenyl, or a C_3-C_6 cycloalkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0368] In certain embodiments of the nineteenth aspect, R^{242} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^{242} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{242} is H. In certain embodiments, R^{242} is a C_1-C_6 alkyl, phenyl, or a C_3-C_6 cycloalkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0369] In certain embodiments of the nineteenth aspect, R^{251} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^{251} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{251} is H. In certain embodiments, R^{251} is a C_1-C_6 alkyl, phenyl, or a C_3-C_6 cycloalkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0370] In certain embodiments of the nineteenth aspect, R^{252} is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN. In certain embodiments, R^{252} is H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl. In certain embodiments, R^{252} is H. In certain embodiments, R^{252} is a C_1-C_6 alkyl, phenyl, or a C_3-C_6 cycloalkyl. The remainder of the variables in formulas (VA)-(VL) are as described above and below with respect to the nineteenth aspect.

[0371] In certain embodiments of the nineteenth aspect,

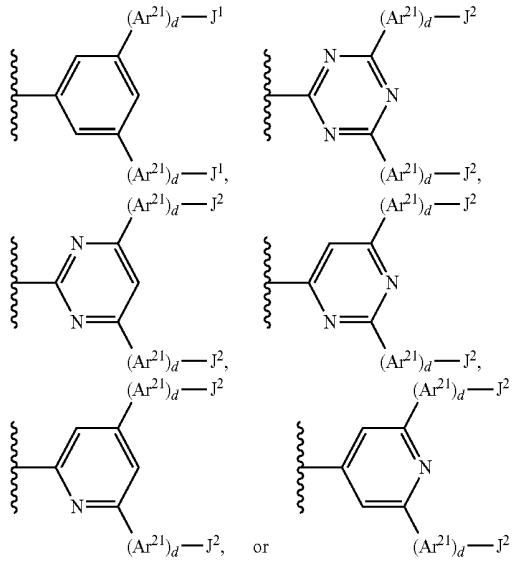
[0372] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H or a C_1-C_6 alkyl;

[0373] R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl;

[0374] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, $—(Ar^{21})_d$-G, or $—Ar^{22}$;

[0375] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls;

[0376] Ar^{22}, for each occurrence independently, is



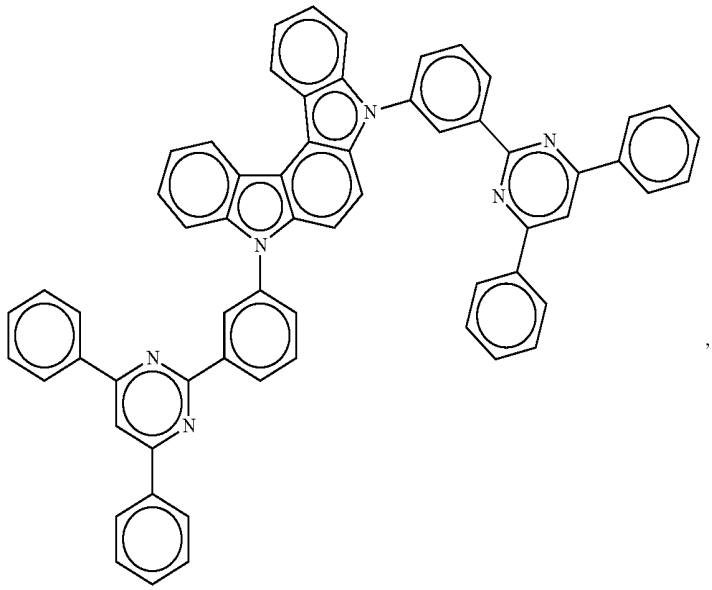
and is optionally substituted with one to three C_1-C_3 alkyls;

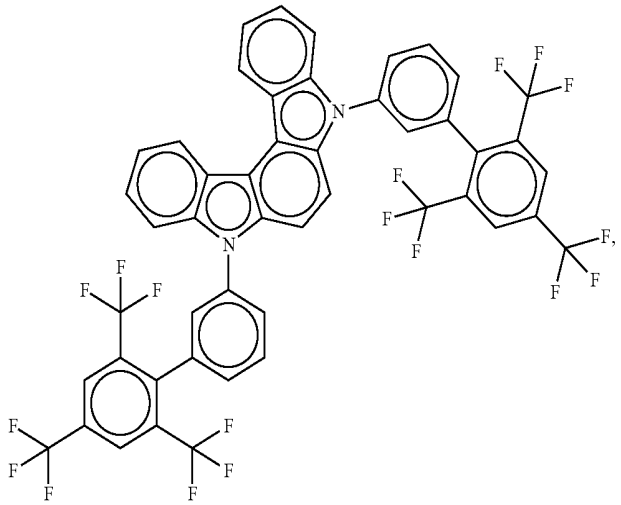
[0377] d, for each occurrence independently, is 0, 1, or 2;

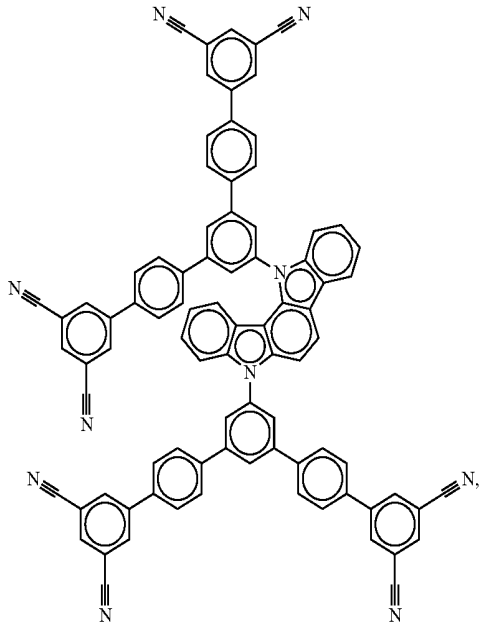
[0378] G, for each occurrence independently, is phenyl substituted with 1, 2, 3, 4, or 5 trifluoromethyls; and

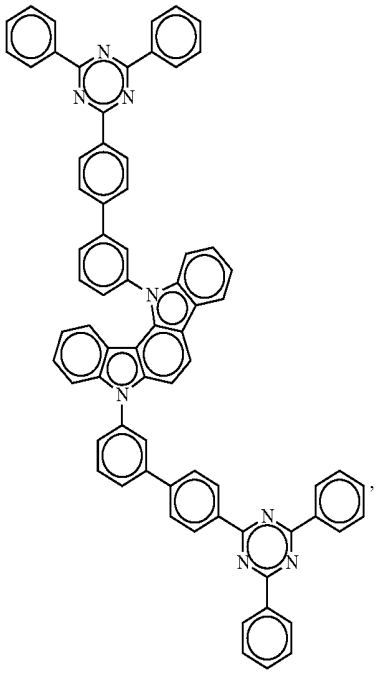
[0379] each occurrence of J^1 or J^2, is independently, phenyl or pyridinyl, and is optionally substituted with 1, 2, 3, 4, or 5 substituents selected from phenyl, trifluoromethyl, or cyano.

[0380] In certain embodiments of the nineteenth aspect, the molecule is represented by one of the following structural formulas:









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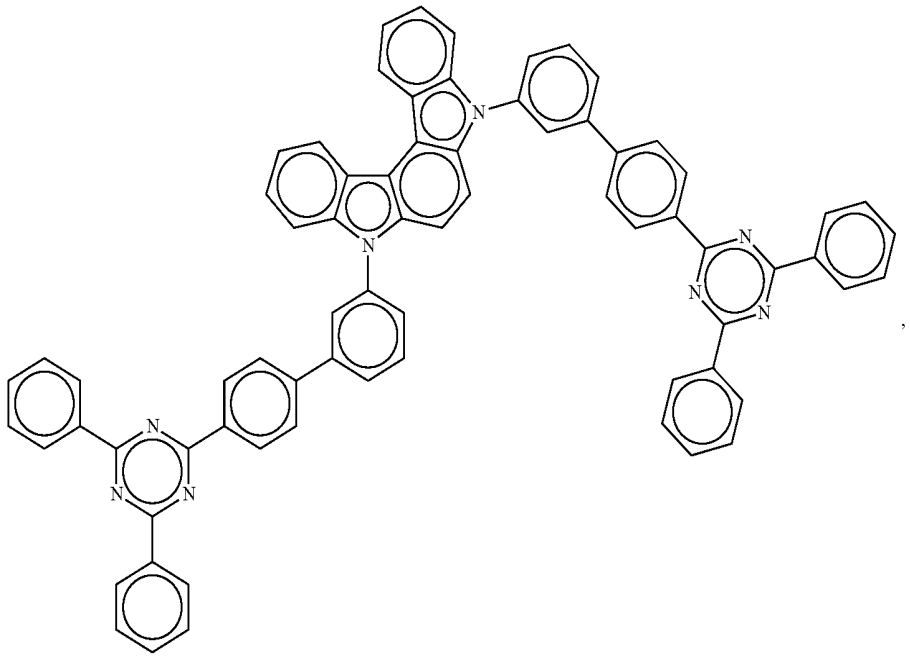

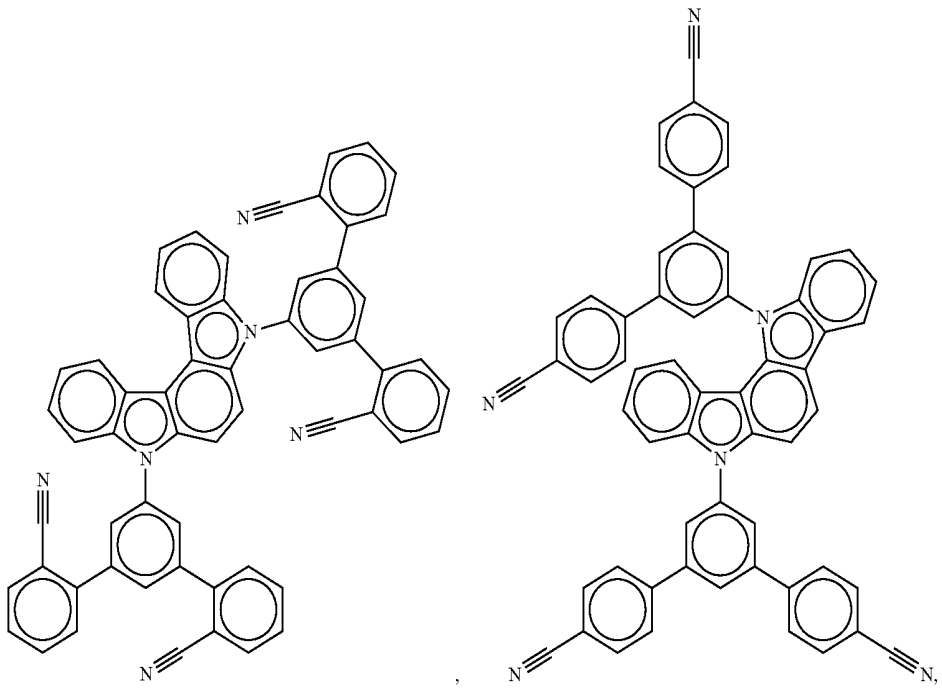

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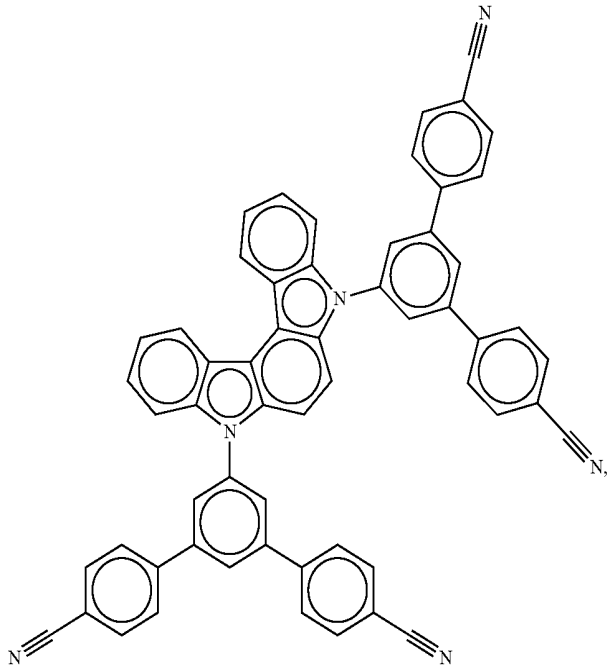

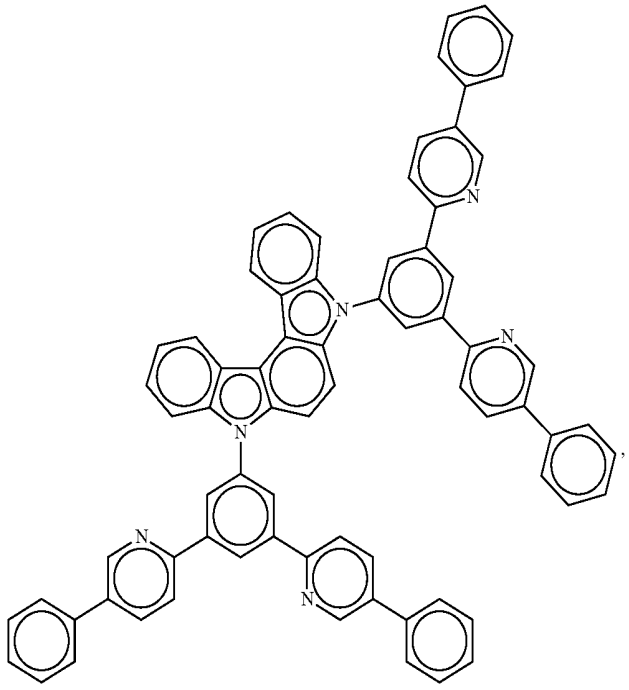

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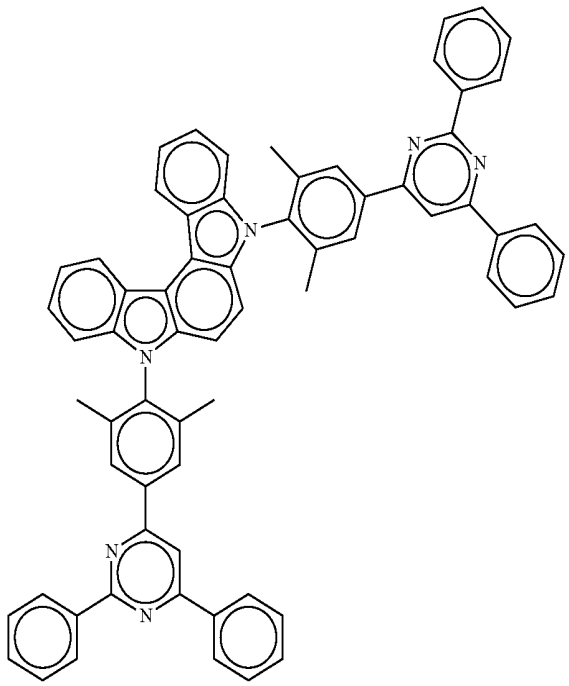

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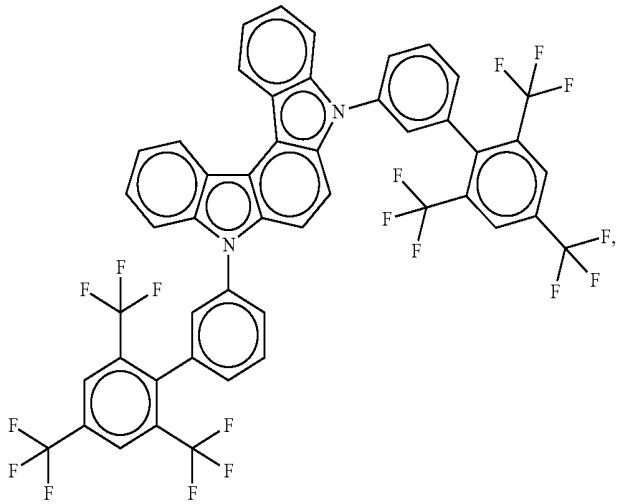

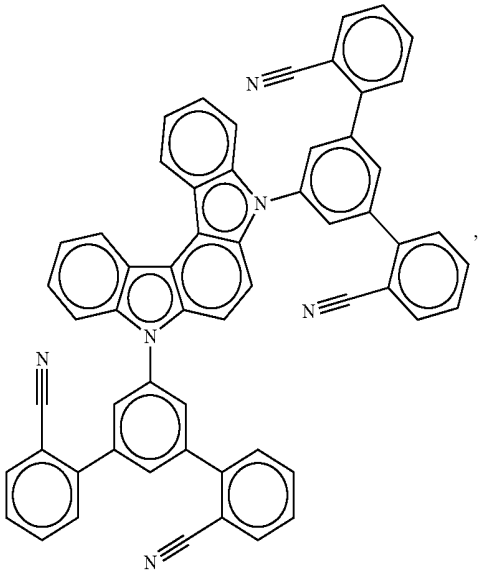

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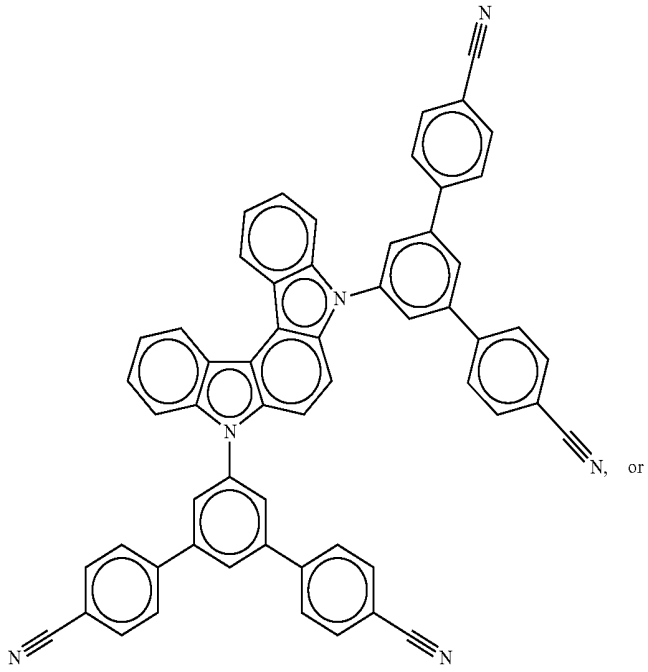

, or

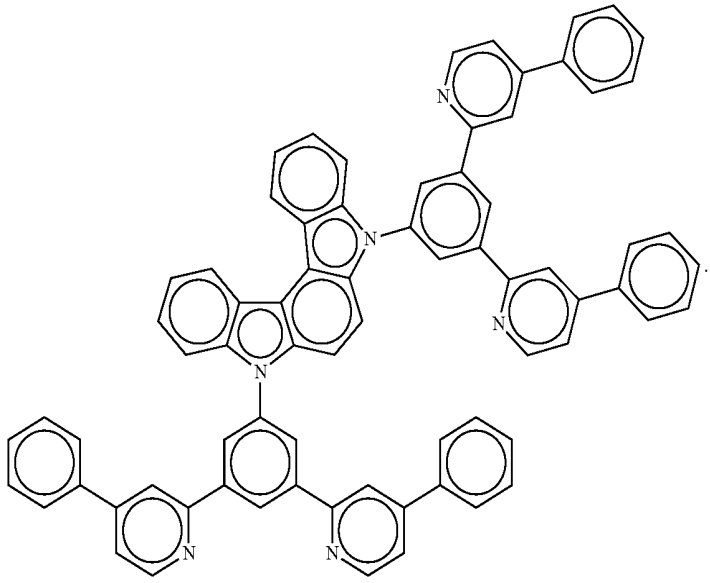

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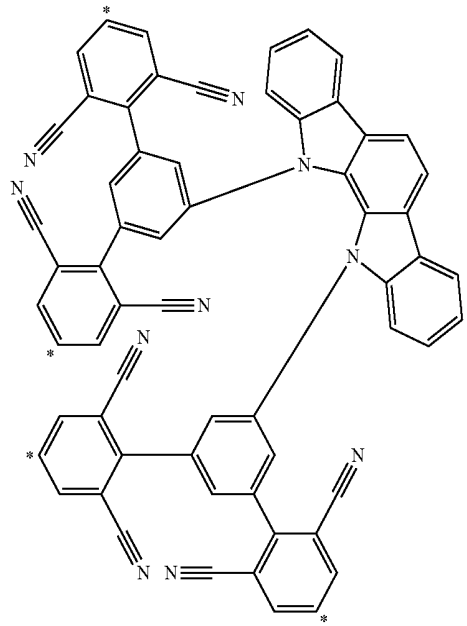
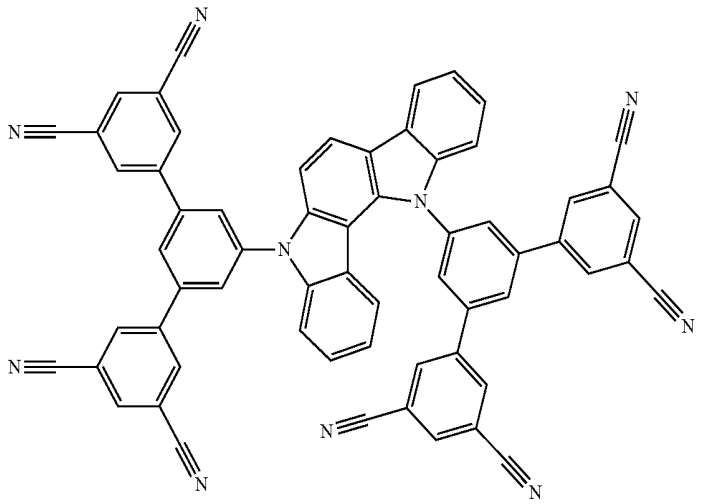
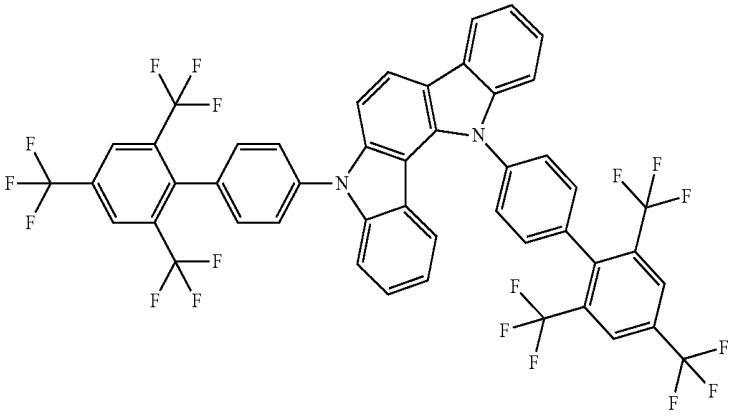
TABLE NR







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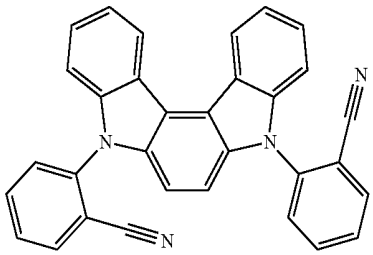

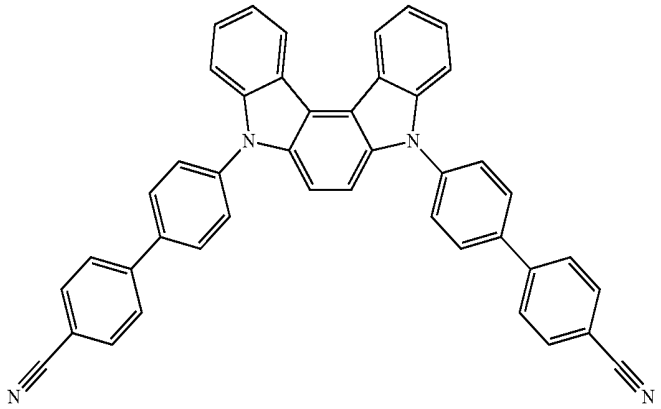

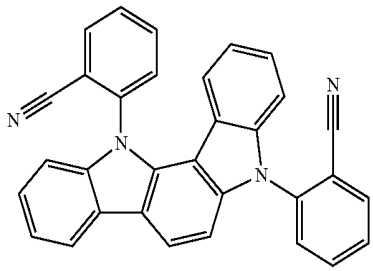

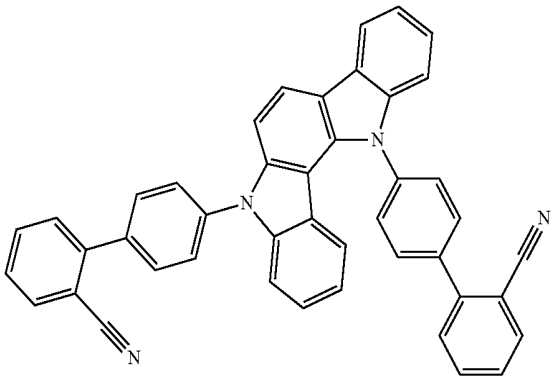

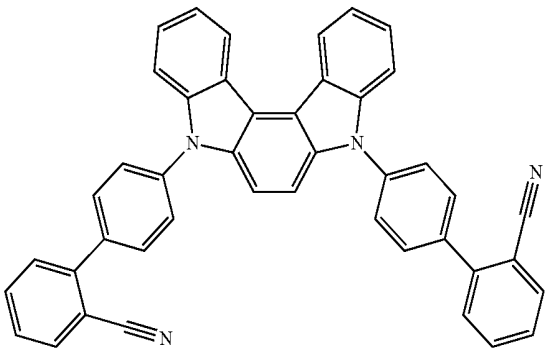

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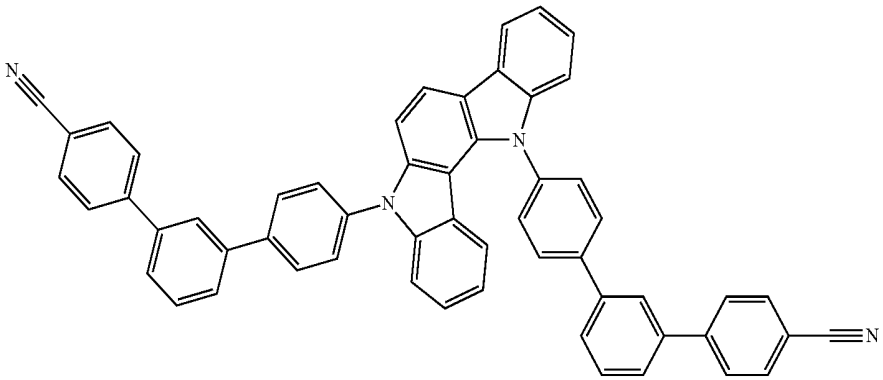
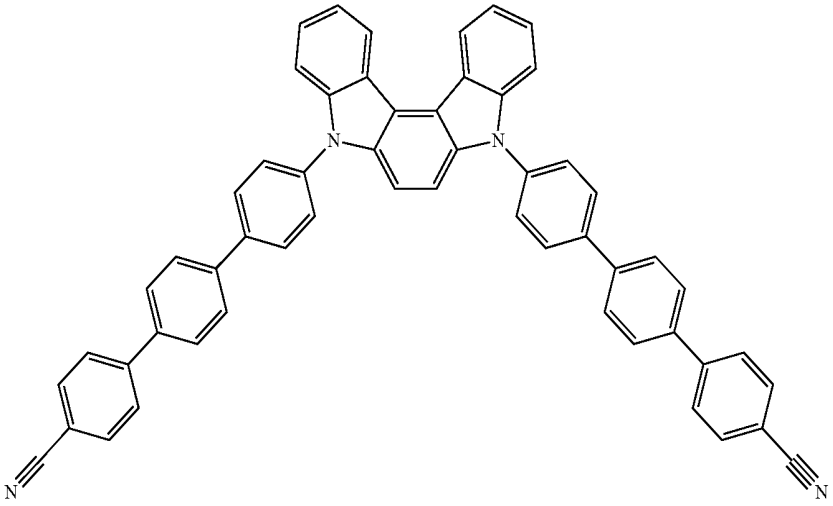
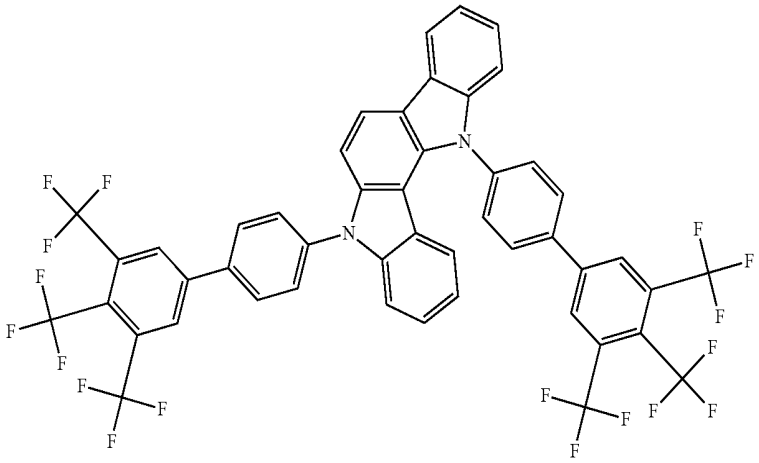
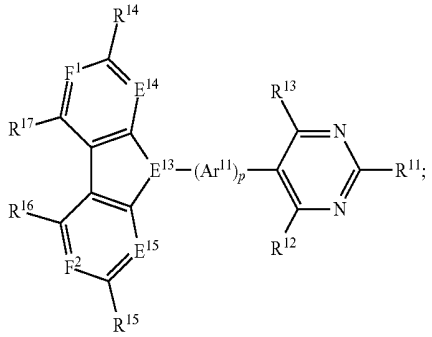






[0381] In a twentieth aspect, the present invention is a molecule represented by structural formula (VI):

(VI)



[0382] In structural formula (VI) of the present invention:

[0383] E^{13} E^{14}, and E^{15} are, each independently, CR^A or N.

[0384] R^A, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0385] At least one of E^{13}, E^{14}, and E^{15} is N.

[0386] R^{11}, R^{12}, and R^{13} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0387] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0388] F^1 is C—$(Ar^{12})_q$-G.

[0389] F^2 is CR^B or N, wherein R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{18}aryl, a 5-20 atom heteroaryl, a halo, or —CN, or —$(Ar^{12})_q$-G.

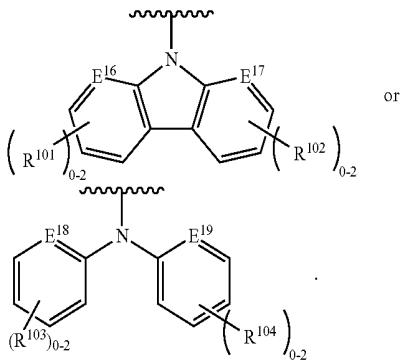
[0390] Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls.

[0391] Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls.

[0392] p is 0, 1, or 2.

[0393] q is 0 or 1.

[0394] G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



or

.

[0395] E^{16}, E^{17}, E^{18}, and E^{19} are, each independently, CR^C or N, wherein R^C is H, a C_1-C_3 alkyl, halo, or —CN.

[0396] R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0397] In one example embodiment of the twentieth aspect, the molecule of structural formula (VI) is not represented by any structural formula in Table 11. In a further example embodiment, in Table 11, each carbon or heteroatom denoted by * in the structural formulas therein is unsubstituted or substituted by a C_1-C_6 alkyl, —OH, —CN, a halo, a C_6-C_{12} aryl, a 5-20 atom heteroaryl, —$N(R^{300})_2$, or —$N(R^{301})_2$, wherein each R^{300}, independently, is H or a C_1-C_6 alkyl and wherein each R^{301}, independently, is H or a C_6-C_{18} aryl.

[0398] In another example embodiment of the twentieth aspect:

[0399] R^{11} is a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0400] Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_2-C_6 alkyls.

[0401] p is 0 or 1.

[0402] Provided that if p is 1, Ar^{11} is unsubstituted phenyl, and R^{11} is unsubstituted phenyl, then F^2 is not CH.

[0403] In an example embodiment of the twentieth aspect:

[0404] R^{11} is C_1-C_6 alkyl or C_6-C_{18} aryl

[0405] R^{12} and R^{13} are, each independently, H, C_1-C_6 alkyl, or C_6-C_{18} aryl.

[0406] In an example embodiment of the twentieth aspect:

[0407] R^{11} is a C_6-C_{18} aryl and R^{12} and R^{13} are, each independently, H or a C_1-C_6 alkyl.

[0408] In an example embodiment of the twentieth aspect:

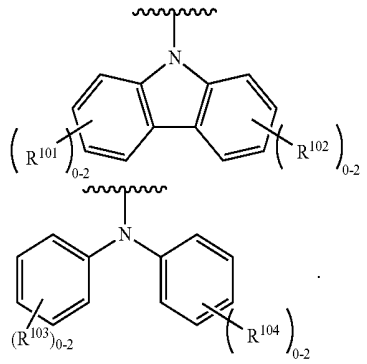
[0409] Ar^{11} is a phenyl.

[0410] In an example embodiment of the twentieth aspect:

[0411] F^2 is CR^B.

[0412] In an example embodiment of the twentieth aspect:

[0413] G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



, or

.

[0414] In an example embodiment of the twentieth aspect:

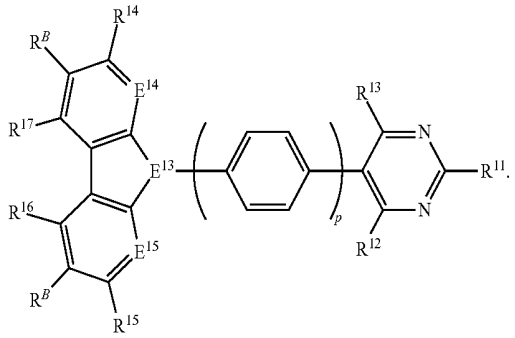
[0415] R^A, for each occurrence independently, is H or a C_1-C_6 alkyl.

[0416] R^{11} is a C_6-C_{18} aryl, and R^{12} and R^{13} are, each independently, H or a C_1-C_3 alkyl.

[0417] R14, $_R{}^{15}$, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl.

[0418] F_1 and F_2 are CR^B wherein R^B is, for each occurrence independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or —$(Ar^{12})_q$-G.

[0419] In an example embodiment of the twentieth aspect, structural formula (I) can be represented by the following structural formula:



[0420] E^{13}, E^{14}, and E^{15}, are, each independently, CR^A or N, wherein R^A, for each occurrence independently, is H or a C_1-C_6 alkyl.

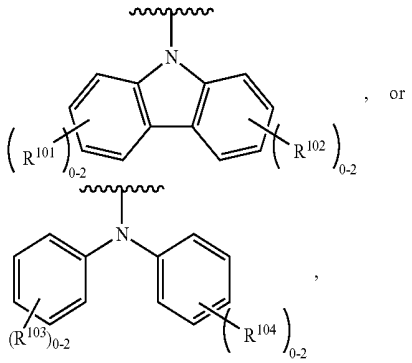
[0421] p is 0 or 1.

[0422] R^{11} is a C_6-C_{18} aryl or a 5-20 atom heteroaryl.

[0423] R^{12} and R^{13} are, each independently, H, a C_1-C_6 alkyl, a halo, or —CN.

[0424] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN.

[0425] R^B is, for each occurrence independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or a moiety represented by one of the following structural formulas:



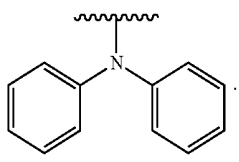
[0426] R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl.

[0427] In an example embodiment of the twentieth aspect:

[0428] E^{13} is N; and

[0429] E^{14} and E^{15} are CR^A.

[0430] In an example embodiment of the twentieth aspect, R^B is, for each occurrence independently, H or a moiety represented by the following structural formula:



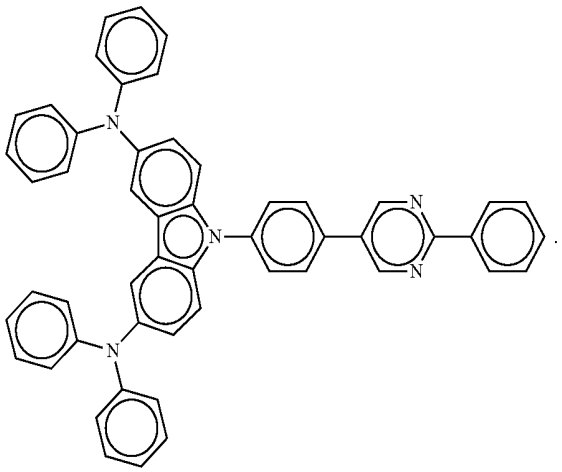
[0431] In an example embodiment of the twentieth aspect:

[0432] R^{11} is a C_6-C_{18} aryl.

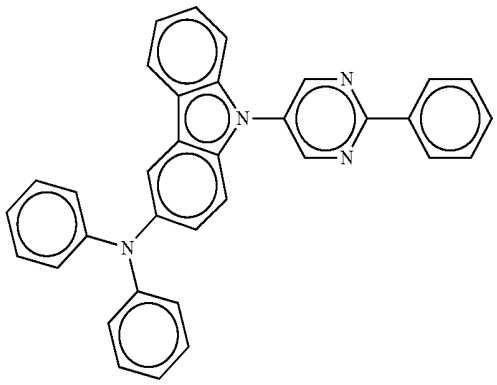
[0433] R^{12} and R^{13} are, each independently, H or a C_1-C_3 alkyl.

[0434] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_{18} cycloalkyl.

[0435] In an example embodiment of the twentieth aspect, molecular structure (VI) can be represented by the following structural formula:

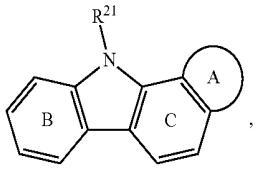


[0436] In an example embodiment of the twentieth aspect, molecular structure (VI) can be represented by the following structural formula:

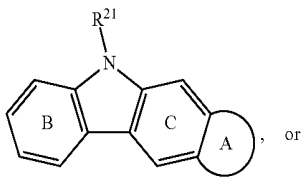


[0437] In a twenty-first aspect, the present invention is a molecule that can be represented by one of structural formulas (VIIA), (VIM), or (VIIC):

(VIIA)



(VIIB)



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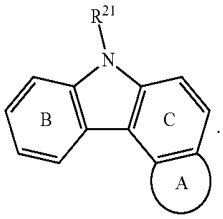
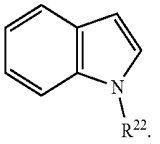
(VIIC)

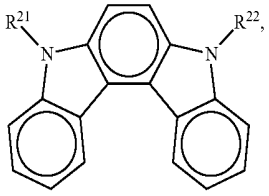


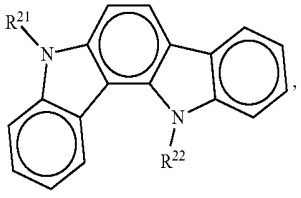
[0438] In structural formulas (VIIA), (VIIB), and (VIIC):

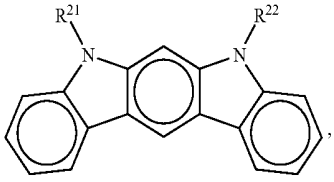
[0439] Ring A, for each occurrence independently, is represented by the following structural formula:

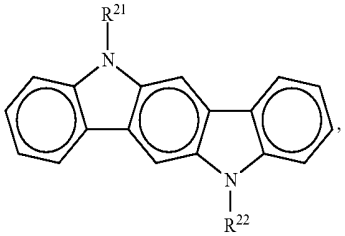


Ring A may be fused to ring C in any orientation. In certain embodiments, any two atoms of the hexacycle of ring A may be shared with ring C. In other embodiments, the two carbon atoms of the pentacycle of ring A may be shared with ring C. In example embodiments, the compounds of structures (VIIA), (VIIB), and (VIIC) can be represented by the following structural formulas:









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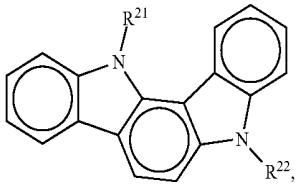

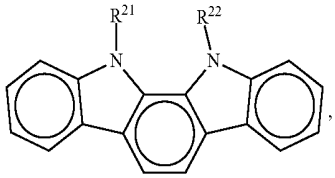

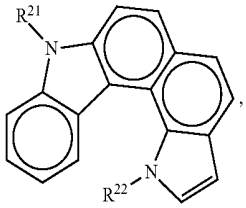

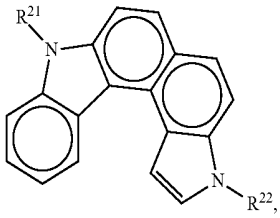

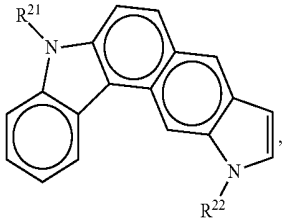

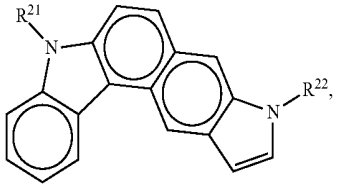

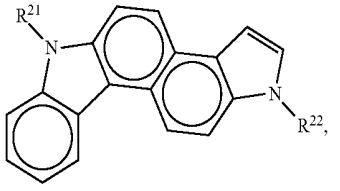

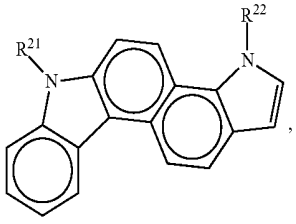

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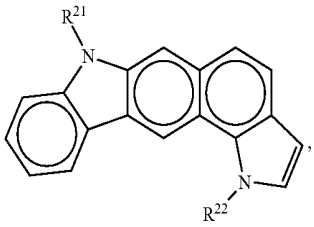

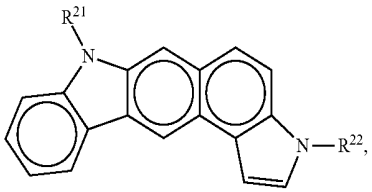

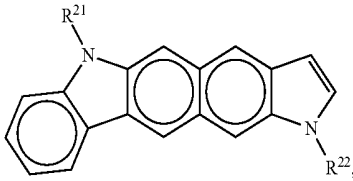

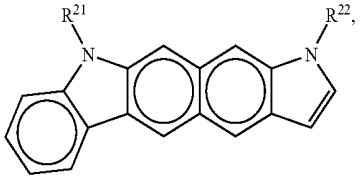

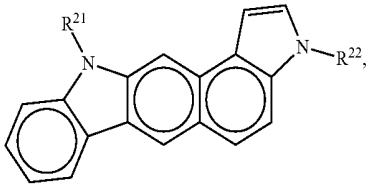

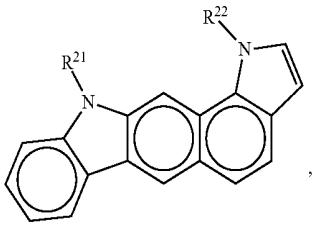

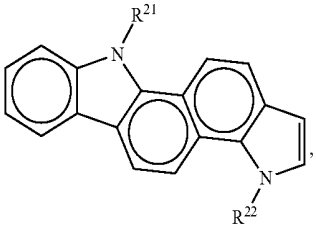

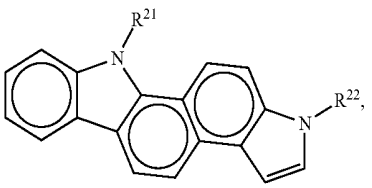

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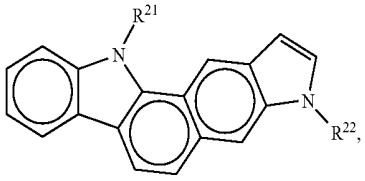
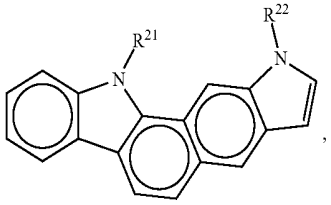
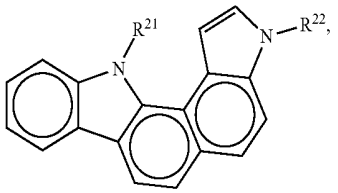
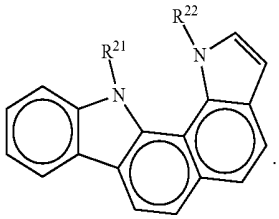








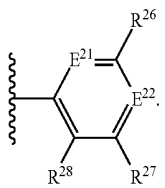
[0440] Rings A, B, and C, each independently, are optionally substituted with 1 to 4 substituents selected from a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0441] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, or $—(Ar^{21})_d$-G. At least one of R^{21} and R^{22} is $—(Ar^{21})_d$-G.

[0442] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls.

[0443] d, for each occurrence independently, is 0, 1, or 2.

[0444] G, for each occurrence independently, is:

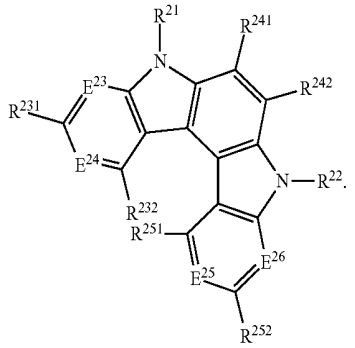


[0445] E^{21} and E^{22} are, each independently, CR^X or N, wherein R^X, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN. At least one of E^{21} and E^{22} is N.

[0446] R^{26}, R^{27}, and R^{28}, for each occurrence independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN.

[0447] In an example embodiment of the twenty-first aspect, the molecule is represented by structural formula (VIID):

(VIID)



[0448] In structural formula (III):

[0449] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0450] R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0451] In an example embodiment of the twenty-first aspect:

[0452] R^{26}, R^{27}, and R^{28} are, each independently, H, C_1-C_6 alkyl, or C_6-C_{18} aryl.

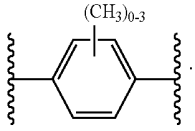
[0453] d is 1 or 2.

[0454] In an example embodiment of the twenty-first aspect:

[0455] R^{26} and R^{27}, each independently, are a C_6-C_{18} aryl, and R^{28} is H or a C_1-C_6 alkyl.

[0456] In an example embodiment of the twenty-first aspect:

[0457] Ar^{21} is a moiety represented by the following structural formula:



[0458] In an example embodiment of the twenty-first aspect:

[0459] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H or a C_1-C_6 alkyl;

[0460] R^{26} and R^{27}, each independently, are a C_6-C_{18} aryl, and R^{28} is H or a C_1-C_3 alkyl; and

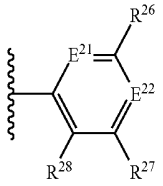
[0461] R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl;

[0462] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or $—(Ar^{21})_d$-G;

[0463] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls;

[0464] d, for each occurrence independently, is 0, 1, or 2;

[0465] G, for each occurrence independently, is:



[0466] E^{21} and E^{22} are, each independently, CR^X or N, wherein R^X, for each occurrence independently, is H, or a C_1-C_6 alkyl.

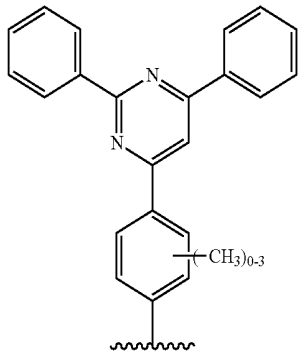
[0467] In an example embodiment of the twenty-first aspect:

[0468] E^{21} and E^{22} are N; and

[0469] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y.

[0470] In an example embodiment of the twenty-first aspect:

[0471] R^{21} and R^{22} are, each independently, selected from H, C_1-C_6 alkyl, C_6-C_{18} aryl, 5-20 atom heteroaryl, or a moiety represented by the following structural formula:



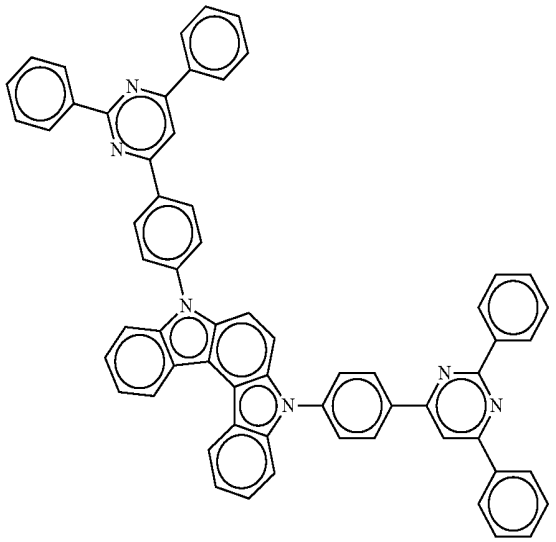
[0472] In an example embodiment of the twenty-first aspect:

[0473] R^{11} is a C_6-C_{18} aryl.

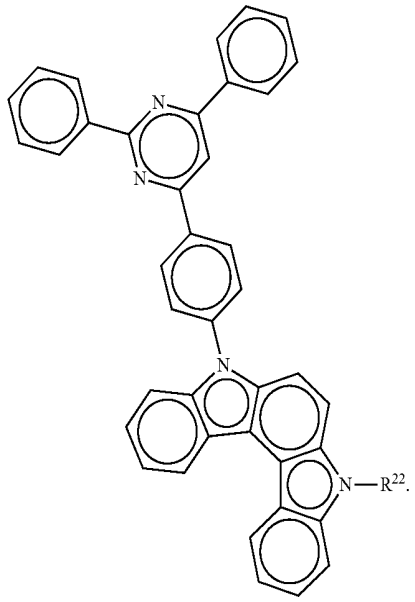
[0474] R^{12} and R^{13} are, each independently, H or a C_1-C_3 alkyl.

[0475] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_{18} cycloalkyl.

[0476] In an example embodiment of the twenty-first aspect, the molecule is represented by the structure:



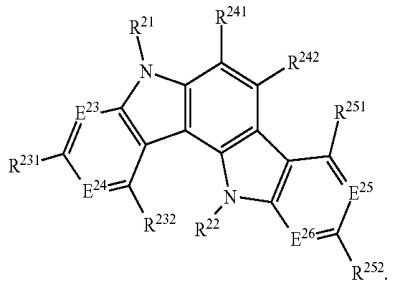
[0477] In another example embodiment of the twenty-first aspect, the molecule is represented by the structure:



[0478] In this structure, R^{22} is H or C_1-C_6 alkyl.

[0479] In an example embodiment of the twenty-first aspect, the molecule is represented by structural formula (VIIE):

(VIIE)



[0480] In structural formula (VIIE):

[0481] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0482] R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0483] In an example embodiment of the twenty-first aspect:

[0484] R^{26}, R^{27}, and R^{28} are, each independently, H, C_1-C_6 alkyl, or C_6-C_{18} aryl.

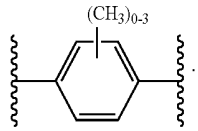
[0485] d is 1 or 2.

[0486] In an example embodiment of the twenty-first aspect:

[0487] R^{26} and R^{27}, each independently, are a C_6-C_{18} aryl, and R^{28} is H or a C_1-C_6 alkyl.

[0488] In an example embodiment of the twenty-first aspect:

[0489] Ar^{21} is a moiety represented by the following structural formula:



[0490] In an example embodiment of the twenty-first aspect:

[0491] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H or a C_1-C_6 alkyl;

[0492] R^{26} and R^{27}, each independently, are a C_6-C_{18} aryl, and R^{28} is H or a C_1-C_3 alkyl; and

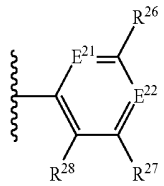
[0493] R231, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl;

[0494] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or $—(Ar^{21})_d$-G;

[0495] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_3 alkyls;

[0496] d, for each occurrence independently, is 0, 1, or 2;

[0497] G, for each occurrence independently, is:



[0498] E^{21} and E^{22} are, each independently, CR^X or N, wherein R^X, for each occurrence independently, is H, or a C_1-C_6 alkyl.

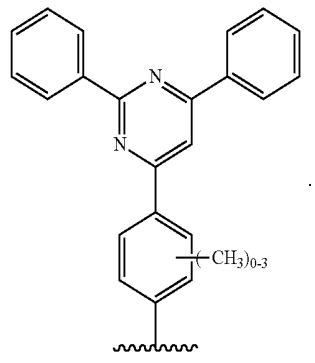
[0499] In an example embodiment of the twenty-first aspect:

[0500] E^{21} and E^{22} are N; and

[0501] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y.

[0502] In an example embodiment of the twenty-first aspect:

[0503] R^{21} and R^{22} are, each independently, selected from H, C_1-C_6 alkyl, C_6-C_{18} aryl, 5-20 atom heteroaryl, or a moiety represented by the following structural formula:



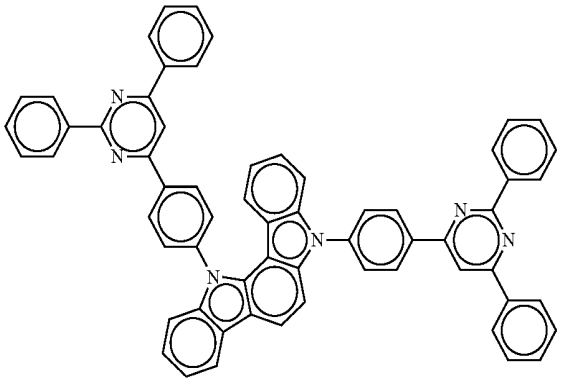
[0504] In an example embodiment of the twenty-first aspect:

[0505] R^{11} is a C_6-C_{18} aryl.

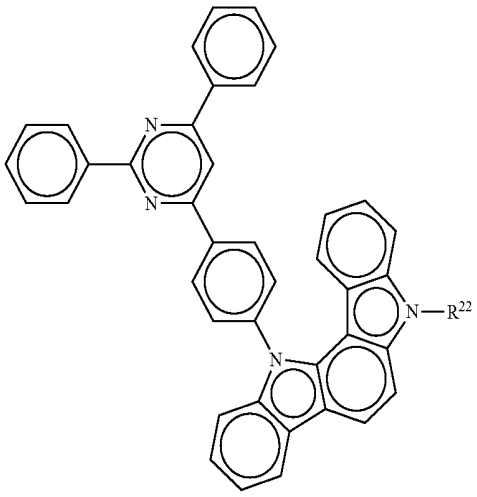
[0506] R^{12} and R^{13} are, each independently, H or a C_1-C_3 alkyl.

[0507] R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_{18} cycloalkyl.

[0508] In an example embodiment of the twenty-first aspect, the molecule is represented by the following structure:



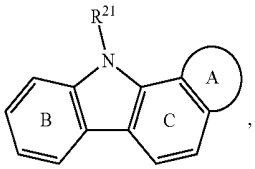
[0509] In another example embodiment of the twenty-first aspect, the molecule is represented by the following structure:



[0510] In this structure, R^{22} is H or C_1-C_6 alkyl.

[0511] In a twenty-second aspect, the present invention is a molecule represented by any one of the following structural formulas:

(VIIIA)



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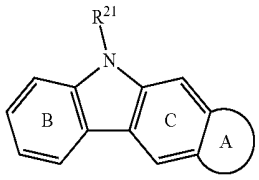
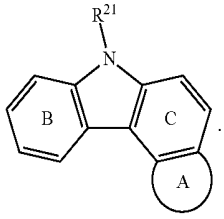
(VIIIB)

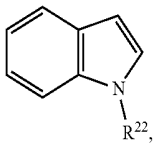


or

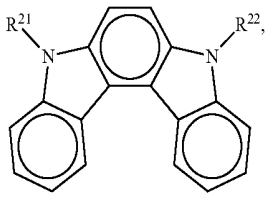
(VIIIC)

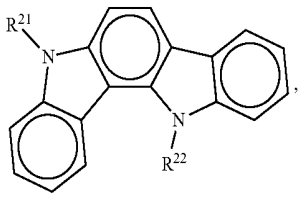


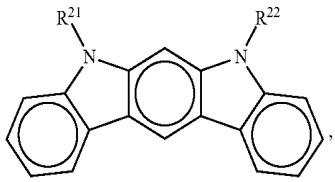
[0512] In structural formulas (VIIIA), (VIIIB), and (VIIIC) of the present invention: Ring A, for each occurrence independently, is represented by the following structural formula:



[0513] Ring A may be fused to ring C in any orientation. In certain embodiments, any two atoms of the hexacycle of ring A may be shared with ring C. In other embodiments, the two carbon atoms of the pentacycle of ring A may be shared with ring C. In example embodiments, the compounds of structures (VIIIA), (VIIIB), and (VIIIC) can be represented by the following structural formulas:







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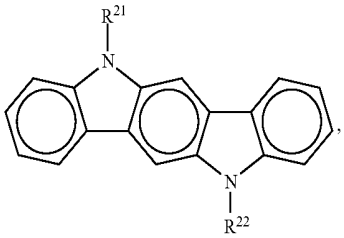

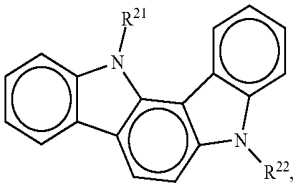

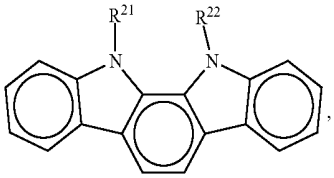

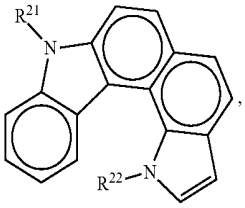

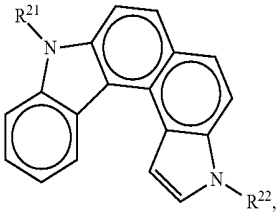

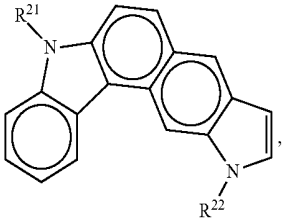

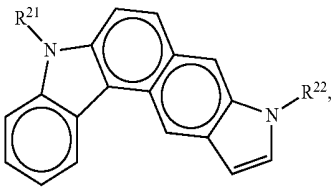

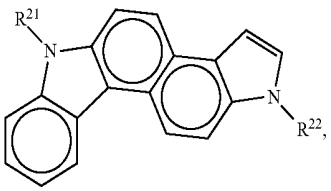

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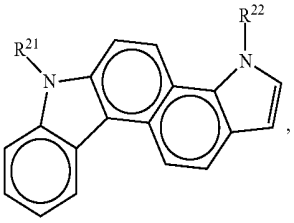

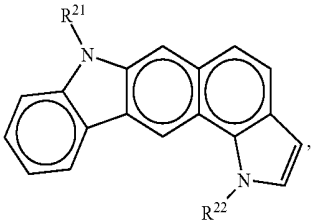

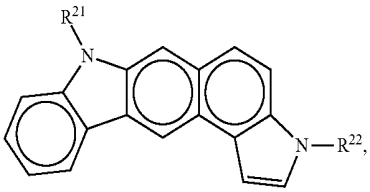

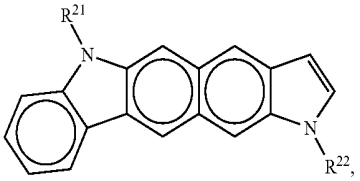

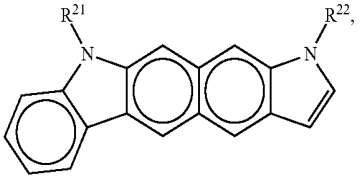

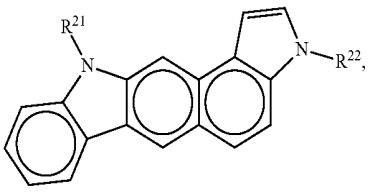

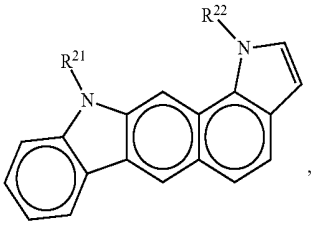

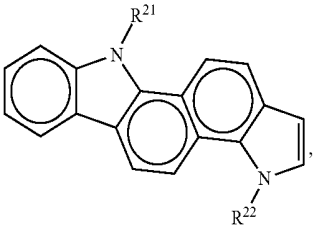

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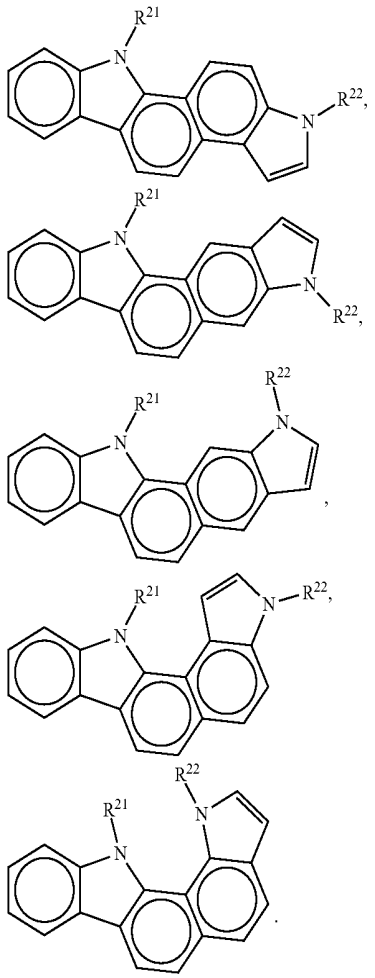
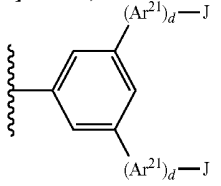


[0514] Rings A, B, and C, each independently, are optionally substituted with 1 to 4 substituents selected from a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0515] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, $—(Ar^{21})_d$-G, or $—Ar^{22}$, provided that at least one of R^{21} and R^{22} is $—(Ar^{21})_d$-G or Ar^{22};

[0516] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0517] Ar^{22}, for each occurrence independently, is:



and is optionally substituted with one to three C_1-C_6 alkyls;

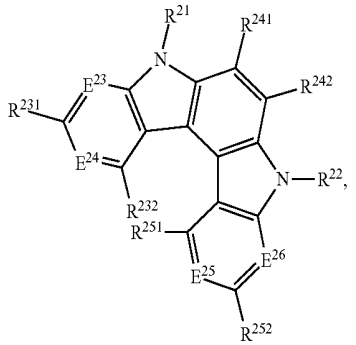
[0518] d, for each occurrence independently, is 0, 1, or 2;

[0519] J, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl, provided that J is not unsubstituted phenyl;

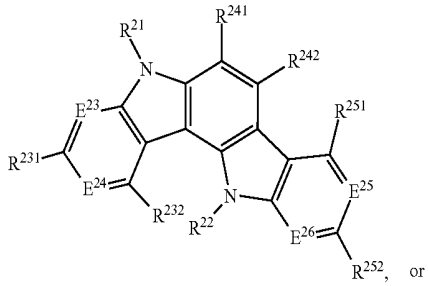
[0520] G, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl, provided that G is not triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl, further provided that if G is phenyl it is not unsubstituted and is not substituted with carbonyl, trifluoromethyl, triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl.

[0521] In an example embodiment of the twenty-second aspect, the present invention is a molecule represented by one of the following structural formulas:

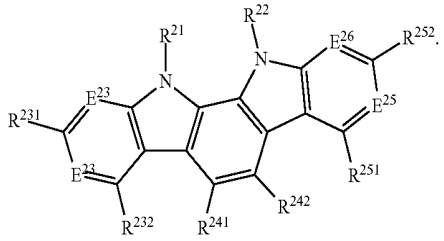
(VIIID)



(VIIIE)



(VIIIF)

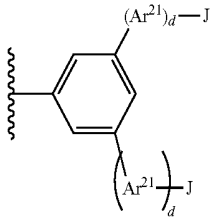


[0522] In structural formulas (VIIIA), (VIIIB), and (VIIIC) of the present invention:

[0523] R^{21} and R^{22}, each independently, are selected from H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, —CN, $—(Ar^{21})_d$-G, or $—Ar^{22}$, provided that at least one of R^{21} and R^{22} is $—(Ar^{21})_d$-G or Ar^{22};

[0524] Ar^{21}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

[0525] Ar^{22}, for each occurrence independently, is:



and is optionally substituted with one to three C_1-C_6 alkyls;

[0526] d, for each occurrence independently, is 0, 1, or 2;

[0527] J, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl, provided that J is not unsubstituted phenyl;

[0528] G, for each occurrence independently, is C_6-C_{18} aryl or 5-20 atom heteroaryl, provided that G is not triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl, further provided that if G is phenyl it is not unsubstituted and is not substituted with carbonyl, trifluoromethyl, triazinyl, pyrimidinyl, tetrazolyl, oxadiazolyl, diazanaphthyl, or pentafluorophenyl;

[0529] E^{23}, E^{24}, E^{25}, and E^{26} are, each independently, CR^Y or N, wherein R^Y, for each occurrence independently, is H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN; and

[0530] R^{231}, R^{232}, R^{241}, R^{242}, R^{251}, and R^{252}, each independently, are H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, halo, or —CN.

[0531] In a twenty-second aspect, the present invention is an organic light-emitting device comprising a first electrode, a second electrode, and an organic layer disposed between the first electrode and the second electrode. In an example embodiment, the organic layer comprises a molecule from any one of the one through eighteen aspects of the present invention described above. In another example embodiment, the organic layer comprises at least one light-emitting molecule represented by a structural formula selected from Table M, N, N', N'', N''', O, Q, Q', B, R, or R'. In yet another example embodiment, the organic layer comprises at least one light-emitting molecule represented by any one of the structural formulas in Table M, N, N', N'', N''', O, Q, Q', B, R, or R'.

[0532] In an example embodiment of any one of the one through twenty-second aspects of the present invention described above, the moiety A and the moiety D are different.

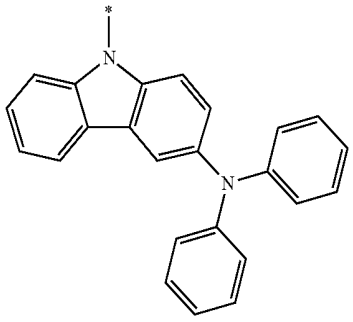
[0533] In an example embodiment of any one of the one through twenty-second aspects of the present invention described above, the moiety D has a highest occupied molecular orbital (HOMO) energy above −6.5 eV and the moiety A has a lowest unoccupied molecular orbital (LUMO) energy below −0.5 eV.

[0534] In an example embodiment of any one of the one through twenty-second aspects of the present invention described above, the molecule is group symmetric or synthetic symmetric.

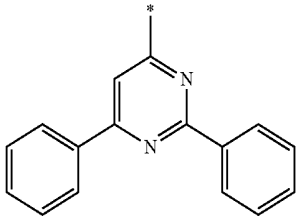
Combinatorial Assembly and Screening

[0535] Example molecules of the present invention having desirable properties, such as color of visible emission, can be constructed from the acceptor, donor, and bridge moieties described above using a combinatorial process described below. While only a few example compounds are illustrated below, it is understood that different combinations of different moieties can be used to create a combinatorial library of compounds. The example moieties below are intended only to illustrate the concepts herein, and are not intended to be limiting.

[0536] In the first step, a library of chemical moieties are screened for their abilities to function as acceptor or donor moieties. Example properties examined include desirable quantum mechanical computations such as the ionization potential of the highest occupied molecular orbital (i.e., a "donor" moiety) and the electron affinity of the lowest unoccupied molecular orbital (i.e., an "acceptor" moiety). In an example embodiment, a donor moiety can be selected if it is calculated that it has an ionization potential of greater than or equal to −6.5 eV. In another example embodiment, an acceptor moiety can be selected if it is calculated that it has an electron affinity of less than or equal to −0.5 eV. An example donor moiety selected after screening could be:

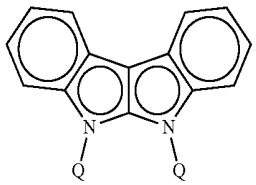


and an example acceptor moiety selected after screening could be:

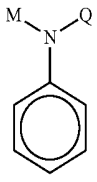


wherein (*) represents a point of attachment for the donor and acceptor moieties either to each other or to a bridge moiety.

[0537] In a second, optional, step, if the selected donor and/or acceptor is "multi-site," the multi-site donor moiety is combined with a single-site bridge moiety, and/or the multi-site acceptor moiety is combined with a single-site bridge moiety. If the donor and/or acceptor moieties are "single-site" moieties, then multi-site bridge moieties can be combined with the selected moieties. For the purposes of the combinatorial assembly, the number of "sites" refers to how many potentially different moieties can be attached. For example, the moiety below has one "site":

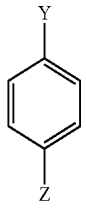


because all moieties attached at the position labeled Q must be the same. Similarly, the moiety below has two "sites" because Q and M can be the same or different:

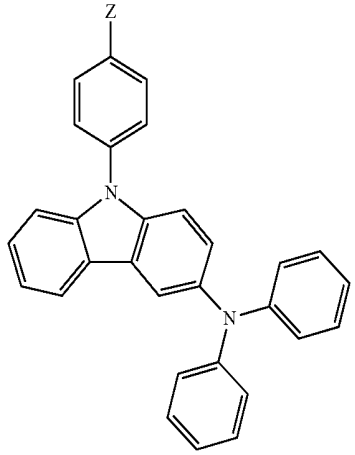


Thus, the nitrogen atom in the molecule is "multi-site."

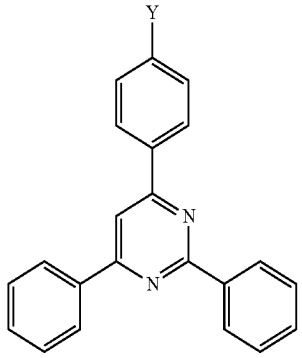
[0538] In the example moieties from the first step, both moieties are single-site. An example "multi-site" bridge could be:



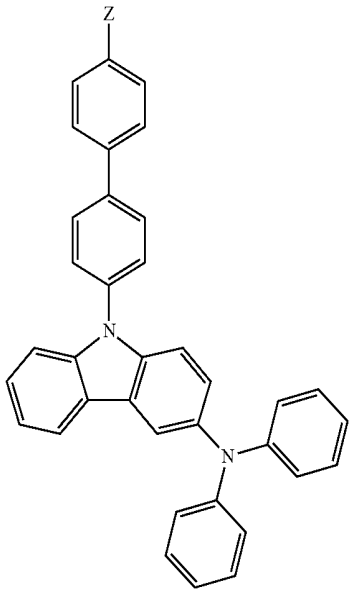
wherein the moieties attached at Y and Z are different. If the donor moiety combines with a bridge, and the acceptor combines with a bridge, the following moieties are created:



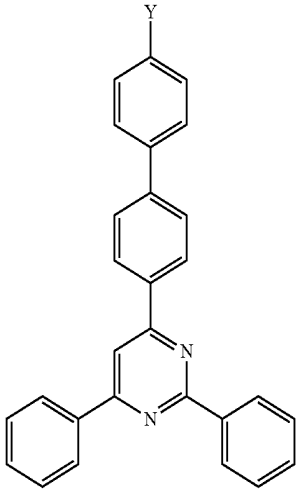
and



[0539] In a third step, the second step can be repeated to continuously add bridge moieties to the molecule. The only limitation is the size of final molecules that are going to be generated. The bridge molecules can be added at position Y or Z, indicated above, and can be the same bridge moiety, or a different bridge moiety. In one example embodiment, the number of bridge moieties can be limited to a number between 0 and 3. In another example, the number of donor moieties and acceptor moieties, or the total molecular weight of the molecule can be limited. In an example embodiment, the molecules are symmetrical. The symmetry can be used to limit the molecules in the combinatorial process to those that are stable. Therefore, for example, an additional bridge moiety added to the moieties from step two could be:

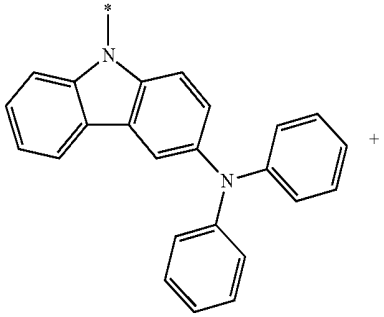


and



[0540] In a fourth step, the unattached point on the bridge moieties only combine with either (1) a donor moiety or an acceptor moiety that does not have a bridge moiety attached; or (2) other bridge moieties that is attached to either an acceptor moiety or a donor moiety such that the size limitation in step three is not violated, and that each molecule comprises at least one donor moiety and one acceptor moiety.

[0541] Using the example moieties and the rules described above, the following example molecules can be created:



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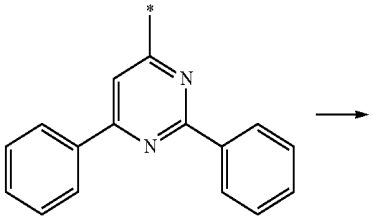

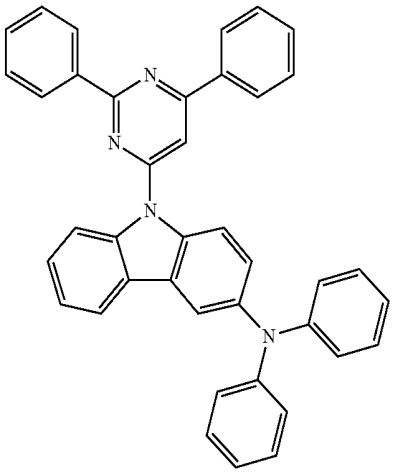

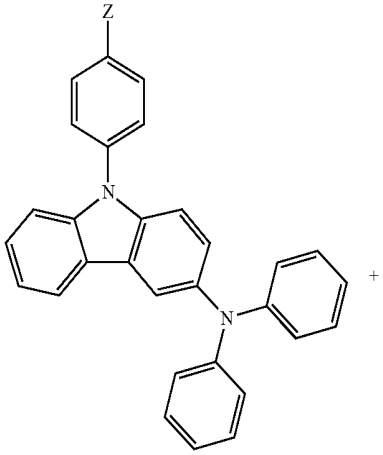

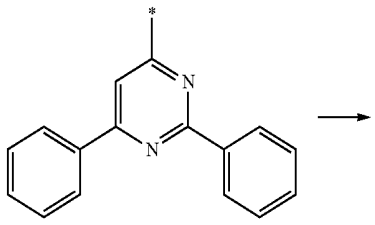

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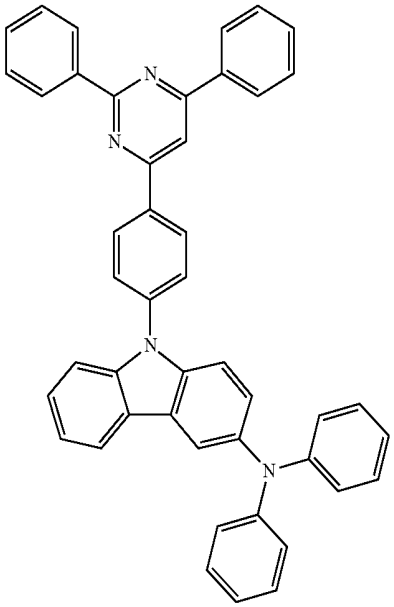

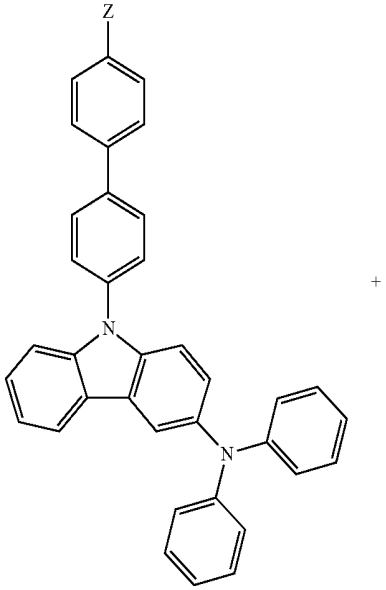

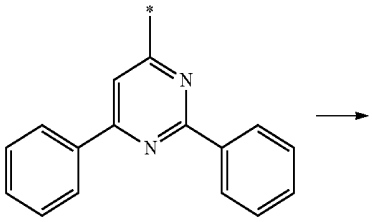

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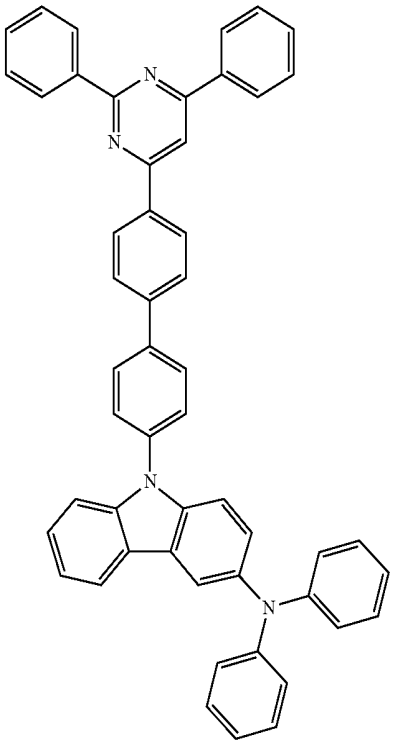


[0542] In the fifth step, the combined potential donors, acceptors, and bridges can be screened based on quantum mechanical computations such as desired HOMO and LUMO values, as well as vertical absorption (the energy required to excite the molecule from the ground state to the excited state), rate of decay (S1 to S0 oscillator strength, e.g., how fast and/or how bright the molecule's emission after excitation), estimated color of visible light emission in nanometers, and the singlet-triplet gap (the energy difference between the lowest singlet excited state, S1, the lowest triplet excited state, T1). Examples of these calculations for molecules embodied in the present invention are provided in Tables 1-10 and 12.

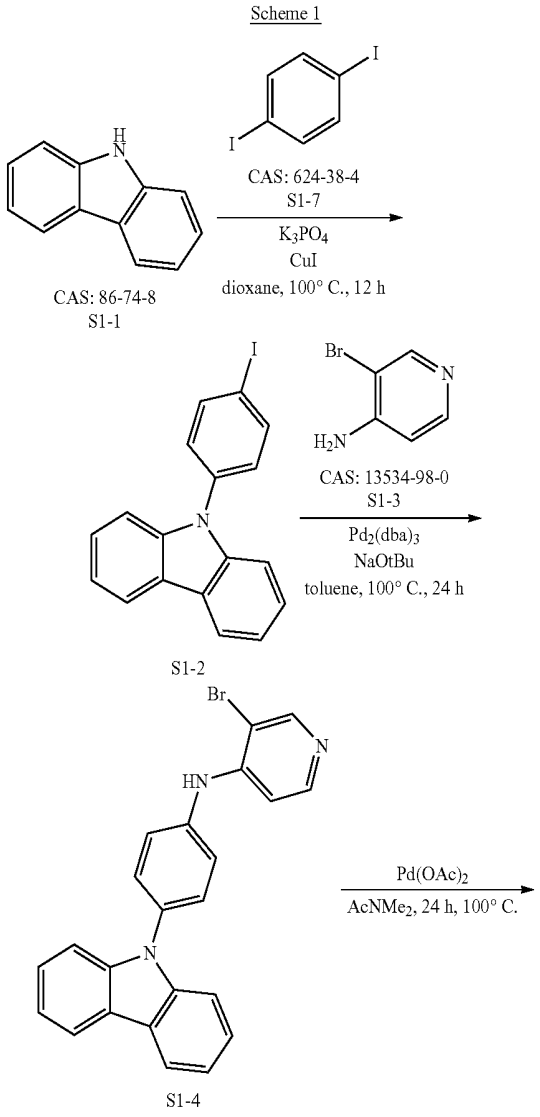
Exemplification

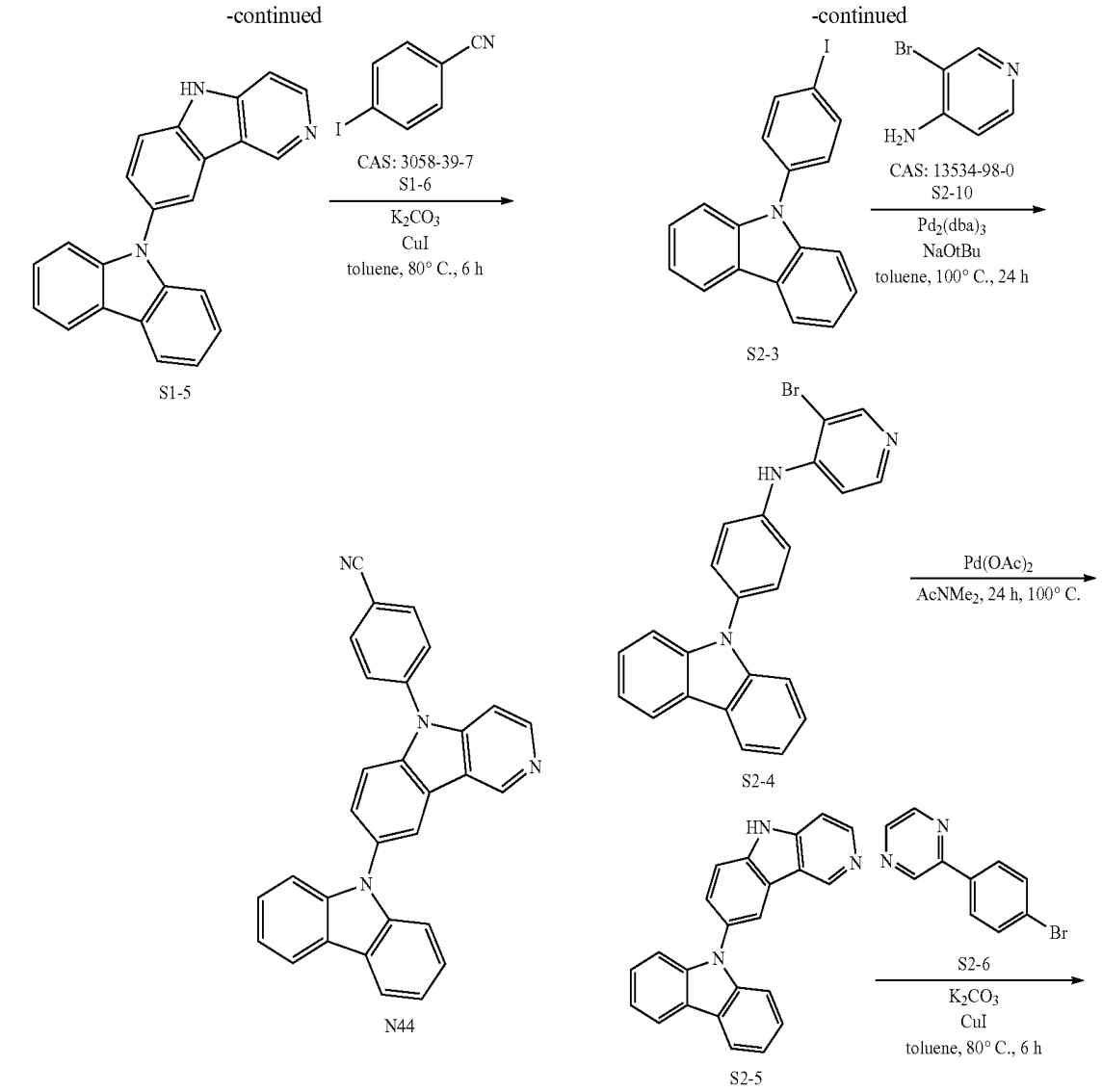
[0543] The compounds described herein may be prepared by synthetic methods known to those of skill in the art. Provided below are exemplary reaction schemes for example embodiments of the present invention. Reactants and conditions suitable for carrying out the reactions described below can be found, for example in: PCT Publication WO2005/070916, Mansanet Ana Maria Castano, et al.; PCT Publication WO2010/050778, Sung Jin Eum et al.; PCT Publication WO2014/021569, Yu-Mi Chang et al.; PCT Publication WO2015/175678; PCT Publication WO2012/080062; U.S. Pat. No. 9,240,559, Oh et al.; U.S. Pat. No. 8,865,322; U.S. Patent Publication 2012/273766; U.S. Patent Publication 2016/006925; European Patent Publication EP2910555; Korean Patent KR101297162; *J. Am. Chem. Soc.* 1984, 106, 2569-2579; *J. Am. Chem. Soc.* 2016, 138, 1709-1716; *J. Am. Chem. Soc.* 2000, 122, 1822-1823; *J. Org. Chem.* 2013, 78, 2639-2648; *J. Org. Chem.* 2002, 67, 7185-7192; *Org. Lett.* 2004, 6, 985-987; *Chem. Commun.* 2015, 51, 12641-12644; *Chem. Commun.* 2012, 48, 5367-5369; *Chem. Commun.* 2014, 50, 13683-13686; *Advanced Synthesis and Catalysis* 2008, 350, 2653-2660; *Org. Lett.* 2004, 6, 985-987; *Org. Lett.* 2004, 6, 985-987; Gu *Angew. Chem. Int. Ed.* 2014, 53, 4850; Stille, J. K. *Angew. Chem. Int. Ed.* 1986, 25, 508; Miyaura, N.; Suzuki, A. *Chem. Rev.* 1995, 95, 2457; *Synthesis* 2005, 4, 547-550; *J. Chem. Soc. Perk.* 2 1985, 705-710; *Synlett* 2013, 24, 603-606; *Advanced Synthesis and Catalysis* 2009, 351, 931-937; *Chem. A Eur. Journal* 2016, 22, 6637-6642; *Chem. A Eur. Journal* 2006, 12, 2222-2234; *Tetrahedron Letters* 2014, 55, 6976-6978; and *J. Organometallic Chem.* 1987, 325, 13-24.

Compound N44

[0544] Compound N44 may be prepared by a person of ordinary skill following Scheme 1. Starting materials S1-1, S1-7, S1-3, and S1-6 are commercially available, for instance from Acros.

Scheme 1

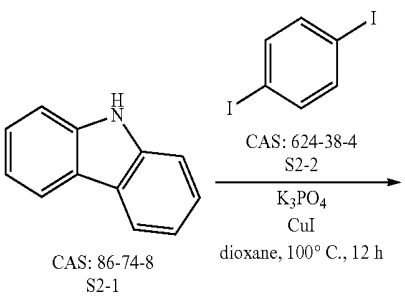


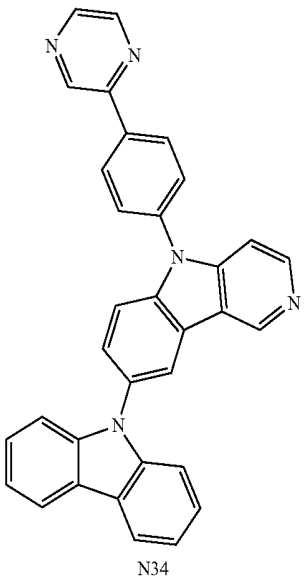


Compound N34

[0545] Compound N34 may be prepared by a person of ordinary skill following Scheme 2. Starting materials S2-1, S2-2, S2-10, S2-8, and S2-9 are commercially available, for instance from Acros or Aldrich.

Scheme 2





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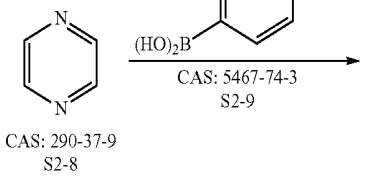

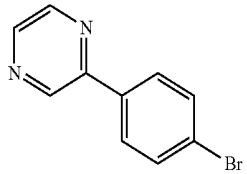

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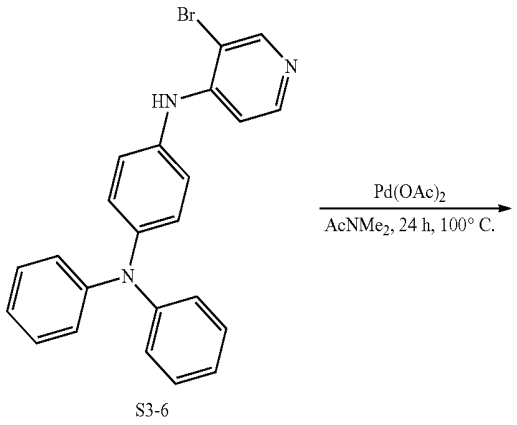
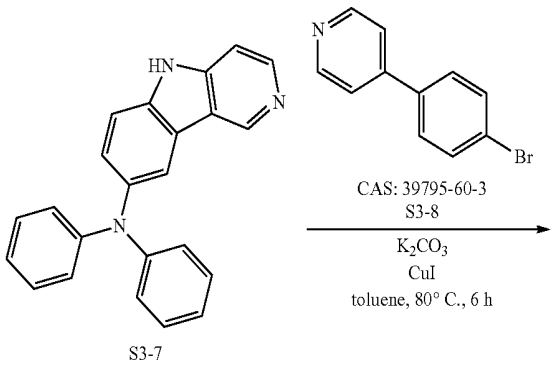
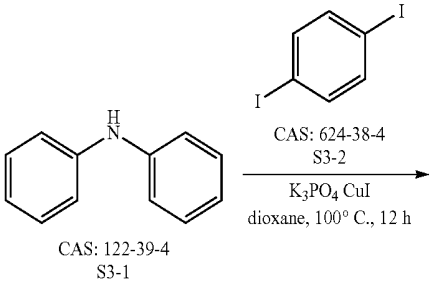


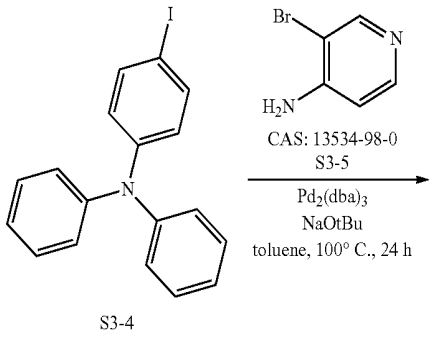
Compound N59

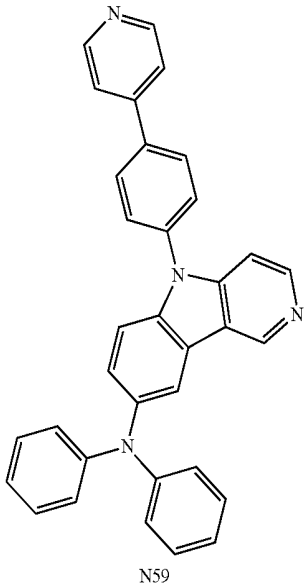
[0546] Compound N59 may be prepared by a person of ordinary skill following Scheme 3. Starting materials S3-1, S3-2, S3-5, and S3-8 are commercially available, for instance from Acros or Arkpharm.



Scheme 3



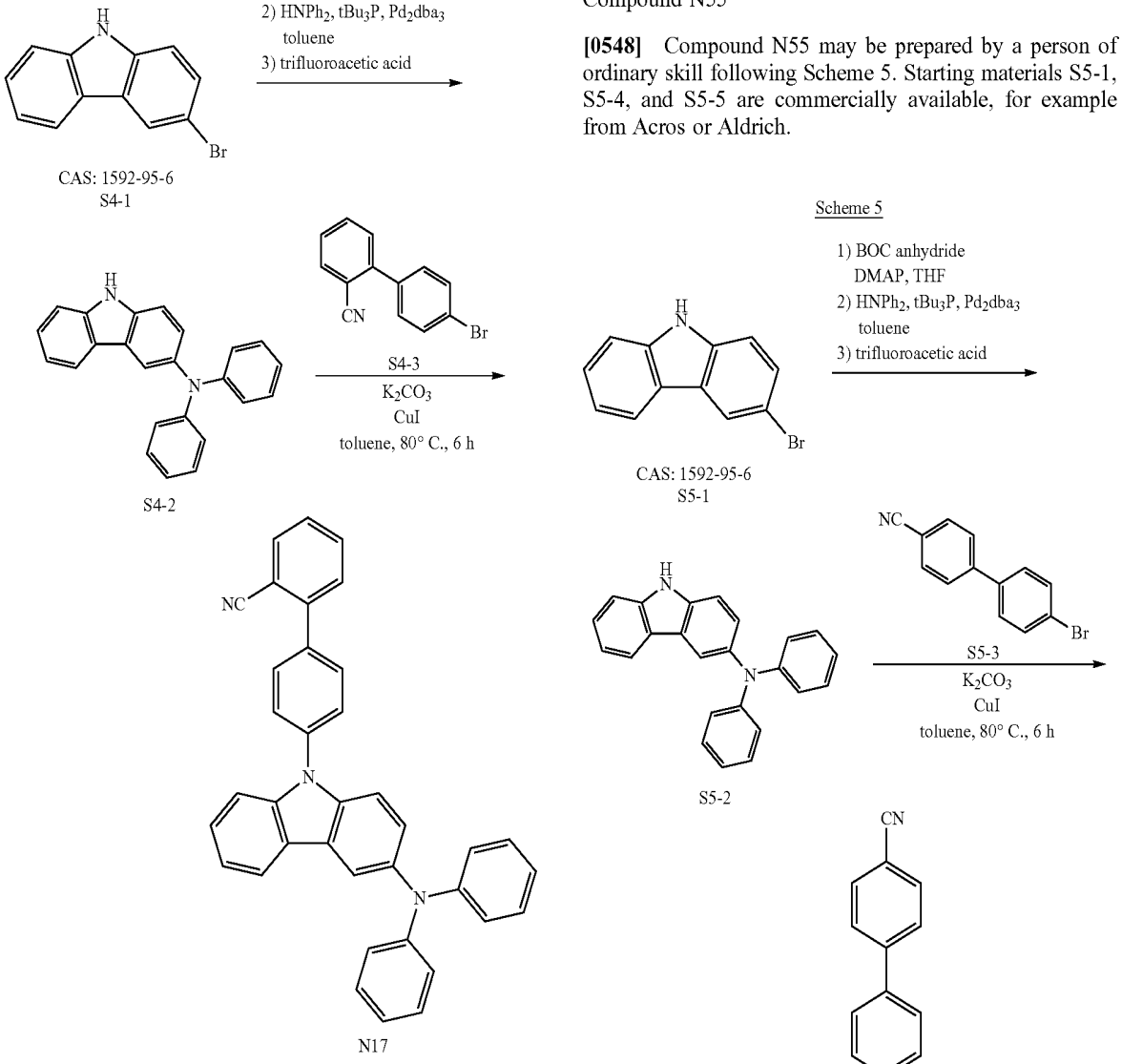




Compound N17

[0547] Compound N17 may be prepared by a person of ordinary skill following Scheme 4. Starting materials S4-1, S4-4, and S4-5 are commercially available, for instance from Acros or Aldrich.

Scheme 4



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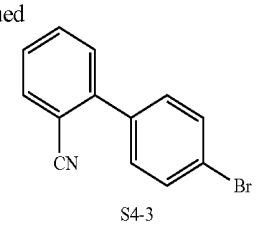


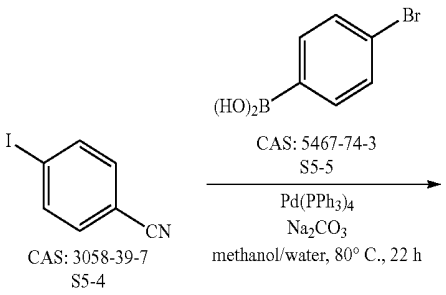
S4-3

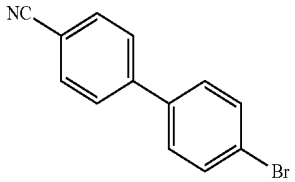
Compound N55

[0548] Compound N55 may be prepared by a person of ordinary skill following Scheme 5. Starting materials S5-1, S5-4, and S5-5 are commercially available, for example from Acros or Aldrich.

Scheme 5

-continued





S5-3

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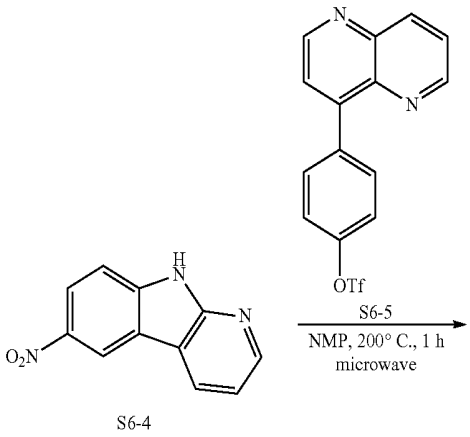
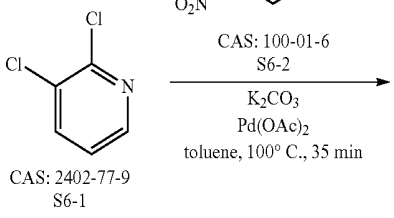


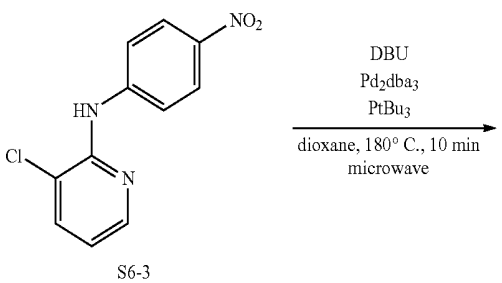
S6-4

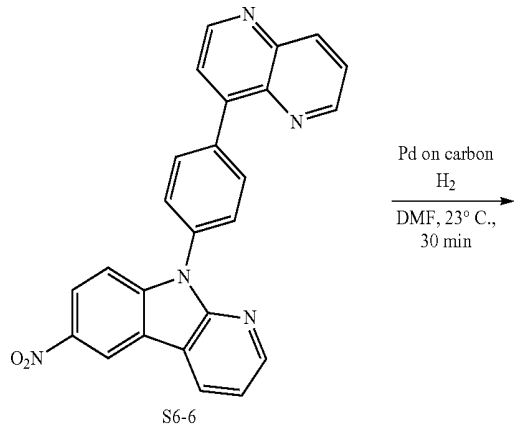
Compound N14

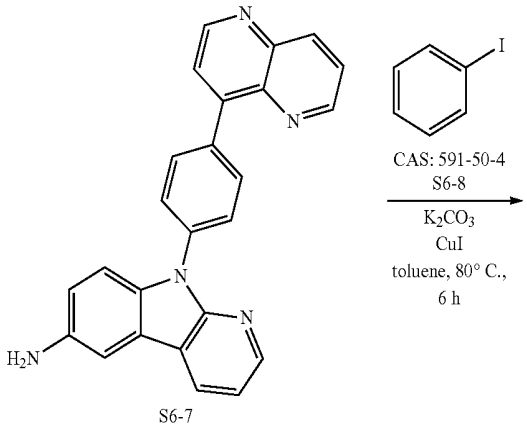
[0549] Compound N14 may be prepared by a person of ordinary skill following Scheme 6. Starting materials S6-1, S6-2, S6-8, S6-9, and S6-10 are commercially available, for instance, from Acros, Aldrich, or Belpharm.

Scheme 6









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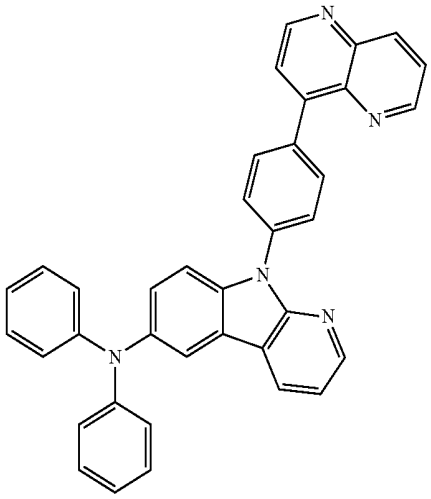
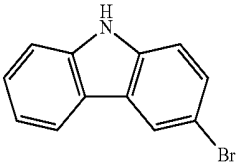


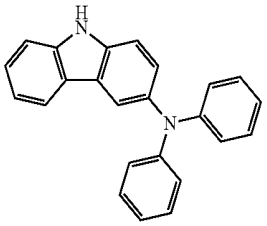
N14

Scheme 7

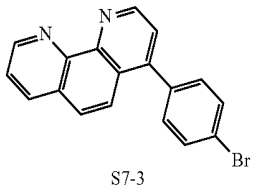


CAS: 1592-95-6
S7-1

1) BOC anhydride
DMAP, THF
2) $HNPh_2$, tBu_3P,
Pd_2dba_3
toluene
3) trifluoroacetic acid

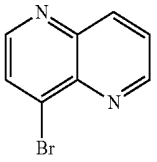


S7-2

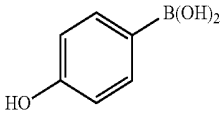


S7-3
K_2CO_3
CuI
toluene, 80° C.,
6 h

Synthesis of fragment:

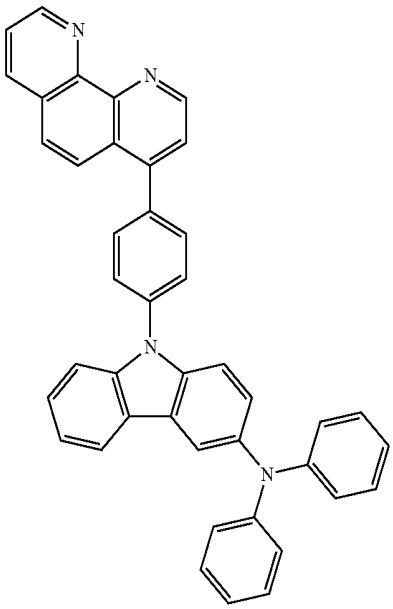


CAS: 9001-34-6
S6-9

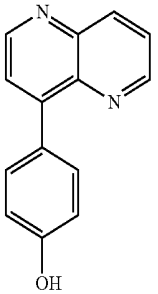


CAS: 71597-85-8
S6-10

$Pd(OAc)_2$, K_3PO_4
THF, 45° C., 24 h
Suzuki cross-coupling

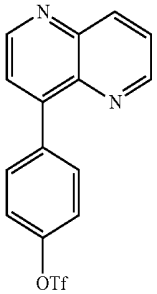


N68



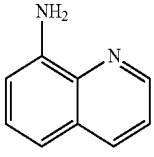
S6-11

Tf_2O
pyridine
DCM, 0° C., 1 h

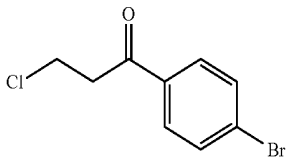


S6-5

Synthesis of fragment:



CAS: 578-66-5
S7-4



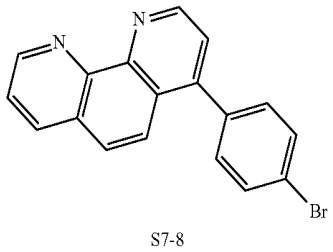
CAS: 31736-73-9
S7-5

H_3PO_4
orthoarsenic acid
120° C., 1.5 h

Compound N68

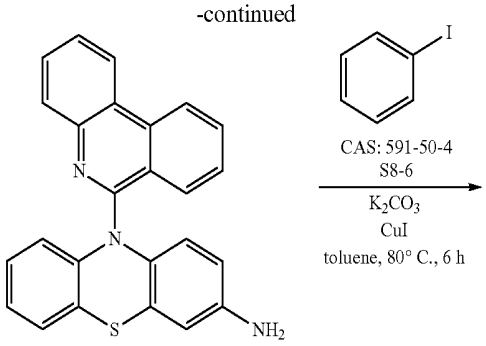
[0550] Compound N14 may be prepared by a person of ordinary skill following Scheme 7. Starting materials S7-1, S7-4, and S7-5 are commercially available, for instance, from Acros or Aldrich.

-continued



S7-8

-continued

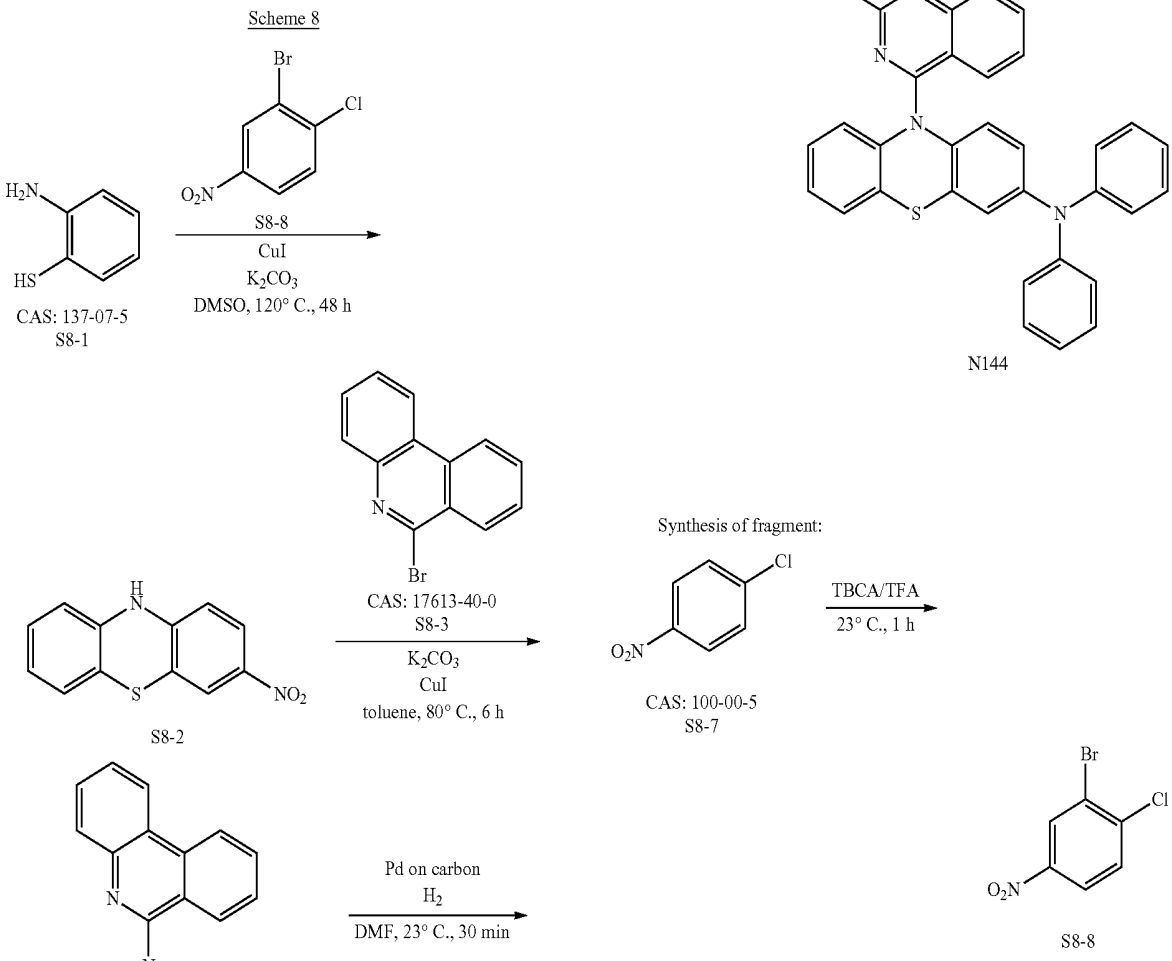


S8-5

Compound N144

[0551] Compound N144 may be prepared by a person of ordinary skill following Scheme 8. Starting materials S8-1, S8-3, S8-6, and S8-7 are commercially available, for instance from Aldrich or Arkpharm.

Scheme 8

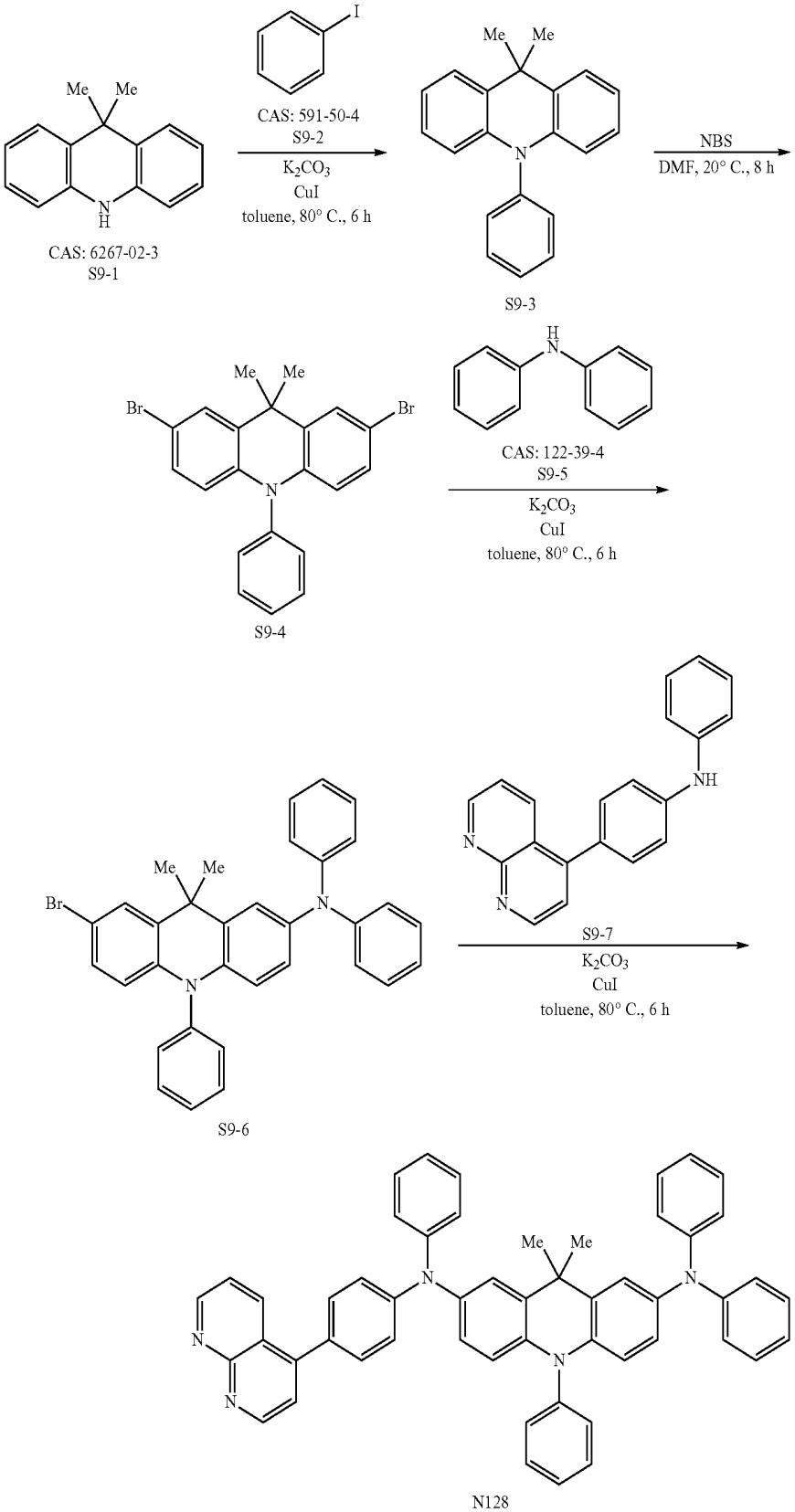


N144

Compound N128

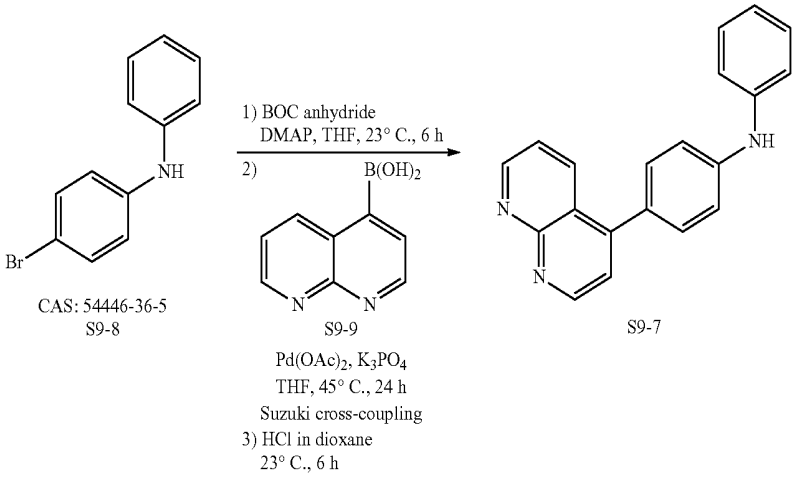
[0552] Compound N128 may be prepared by a person of ordinary skill following Scheme 9. Starting materials S9-1, S9-2, S9-5, S9-8, S9-9 are commercially available, for example, from ArkPharm, Aldrich, or Acros.

Scheme 9


Me
Me
N
H
CAS: 6267-02-3
S9-1
I
CAS: 591-50-4
S9-2
K_2CO_3
CuI
toluene, 80° C., 6 h
Me
Me
N
S9-3
NBS
DMF, 20° C., 8 h
Br
Br
S9-4
H
N
CAS: 122-39-4
S9-5
K_2CO_3
CuI
toluene, 80° C., 6 h
S9-6
NH
S9-7
K_2CO_3
CuI
toluene, 80° C., 6 h
N128

-continued

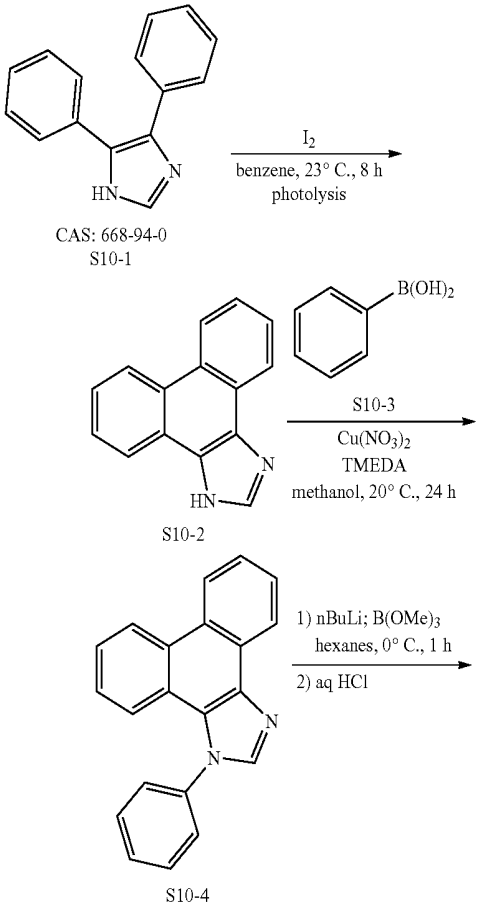
Synthesis of fragment:



Compound N53

[0553] Compound N53 may be prepared by a person of ordinary skill following Scheme 10. Starting materials S10-1, S10-3, and S10-7 are commercially available, for instance from Aldrich or Arkpharm.

Scheme 10



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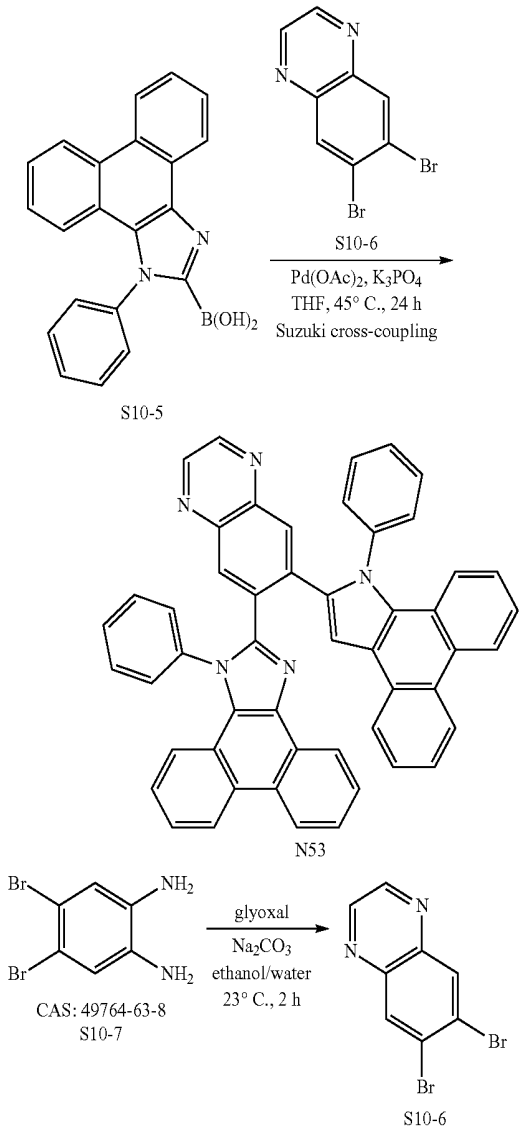
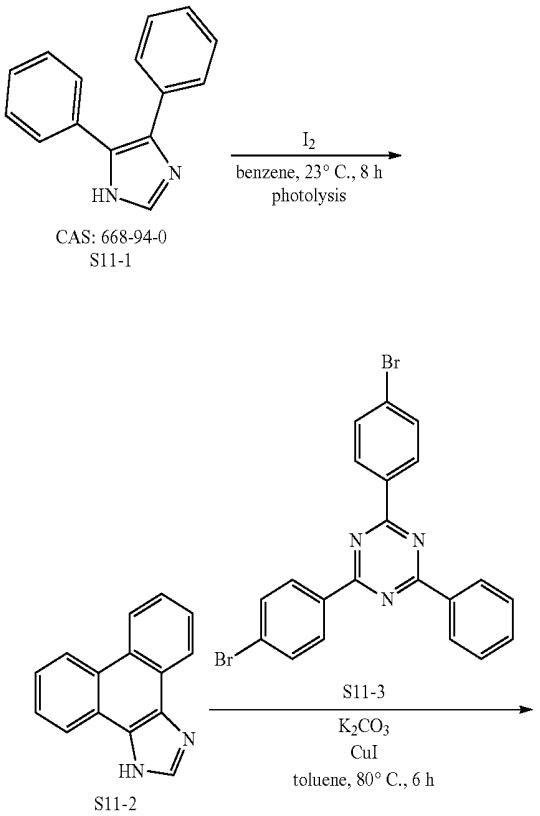


Compound N92

[0554] Compound N92 may be prepared by a person of ordinary skill following Scheme 11. Starting materials S11-1, S11-4, and S11-5 are commercially available, for instance from Aldrich.

Scheme 11



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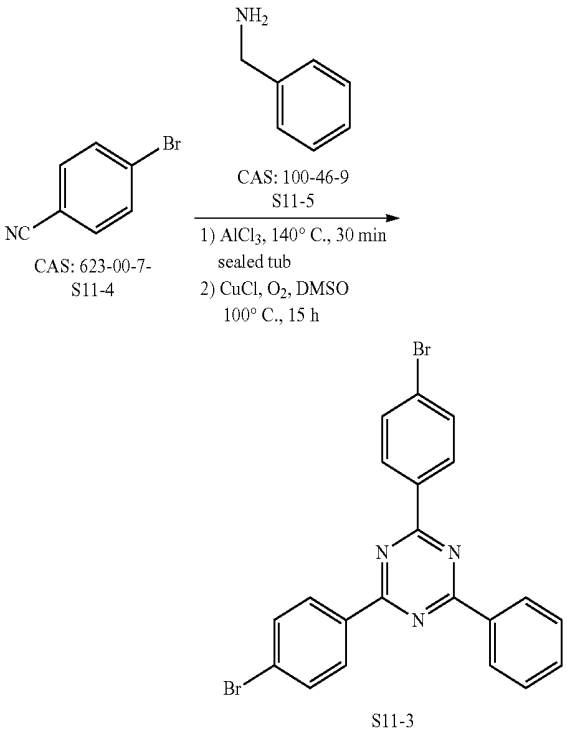
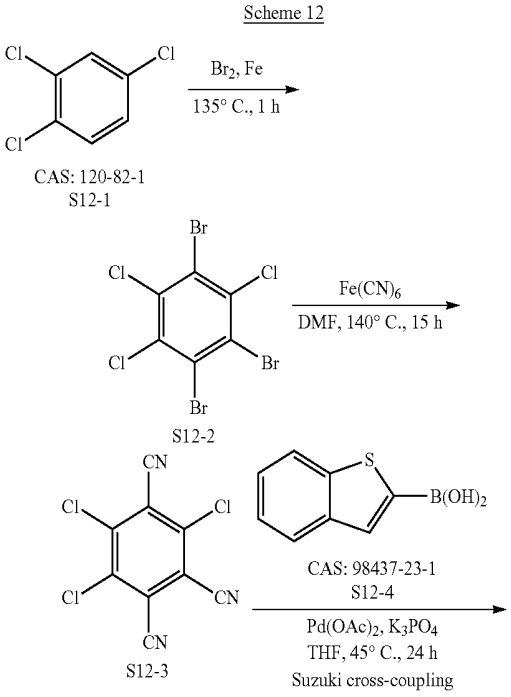
Synthesis of fragment:



Compound Q11

[0555] Compound Q11 may be prepared by a person of ordinary skill following Scheme 12. Starting materials S12-1 and S12-4 are commercially available and may be purchased, for example, from Acros or Aldrich.

Scheme 12



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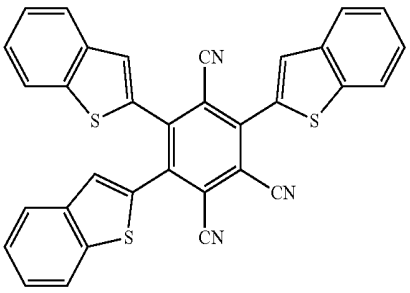
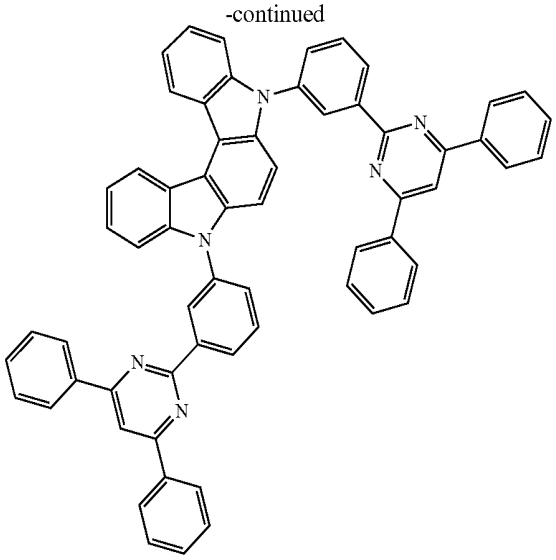


Q11

Compound R19

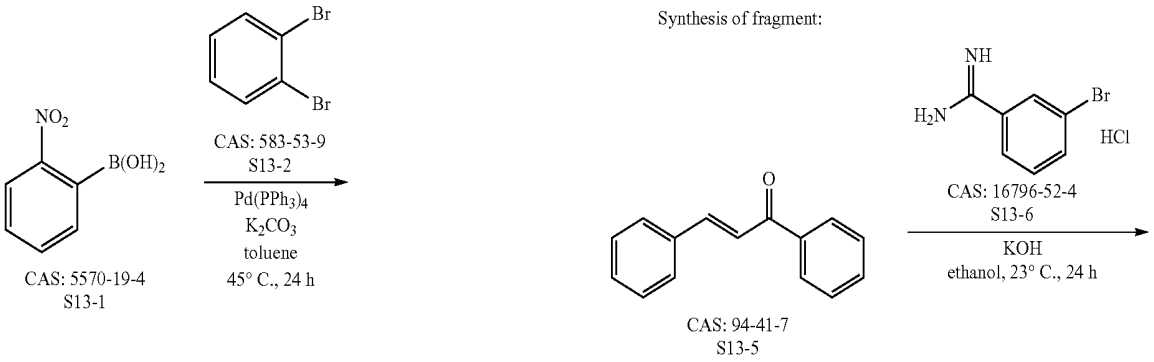
[0556] Compound R19 may be prepared by a person of ordinary skill following Scheme 13. Starting materials S13-1, S13-2, and S13-5 are commercially available, for instance, from Acros or Aldrich.

-continued



R19

Scheme 13

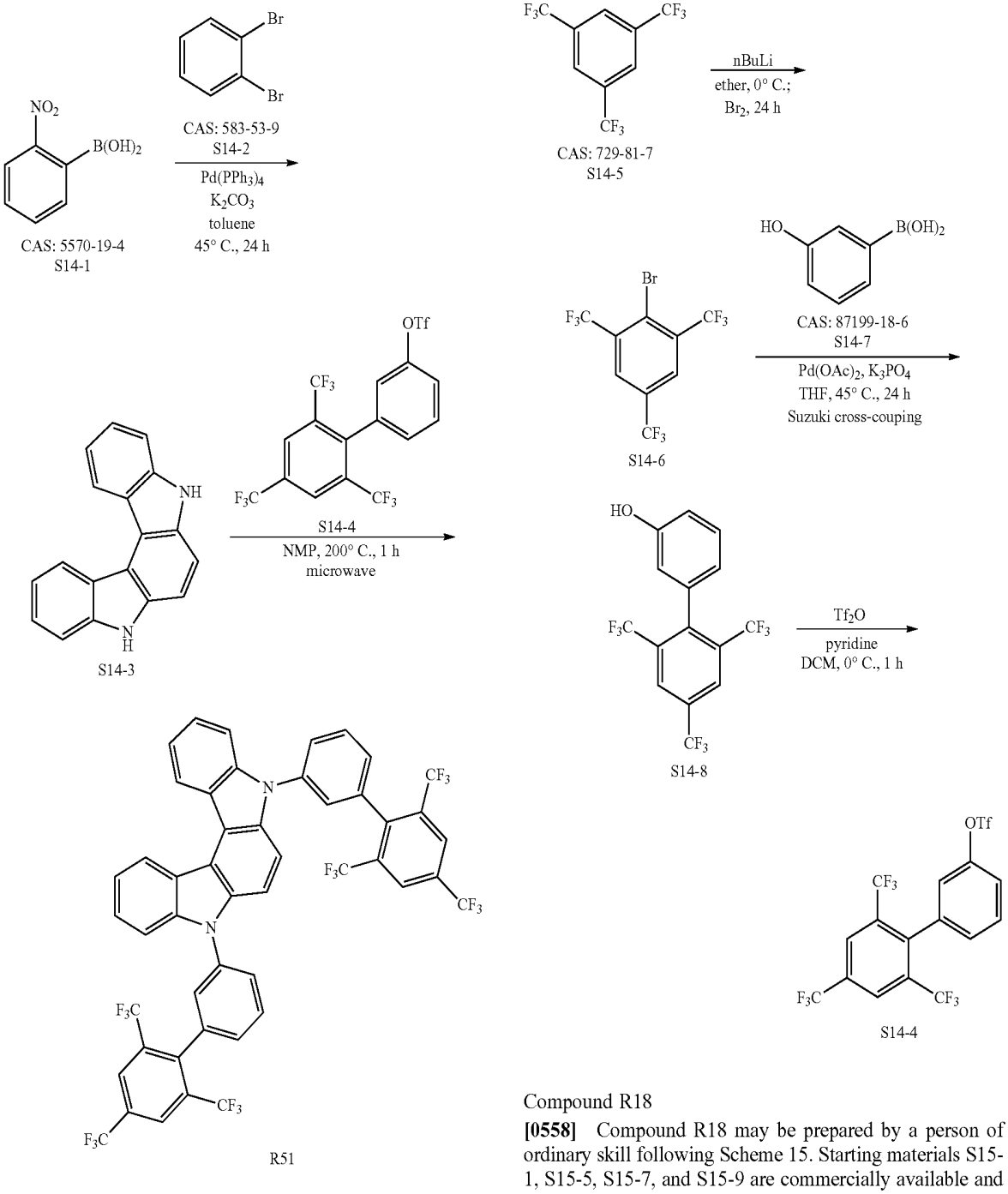


Compound R51

[0557] Compound R51 may be prepared by a person of ordinary skill following Scheme 14. Starting materials S14-1, S14-2, S14-5, and S14-7 are commercially available, for example, from Acros or Aldrich.

-continued

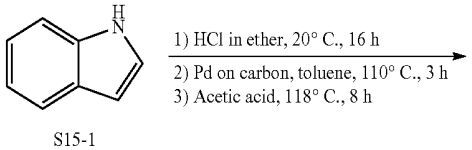
Scheme 14



Compound R18

[0558] Compound R18 may be prepared by a person of ordinary skill following Scheme 15. Starting materials S15-1, S15-5, S15-7, and S15-9 are commercially available and may be purchased, for example, from Acros or Aldrich.

Scheme 15



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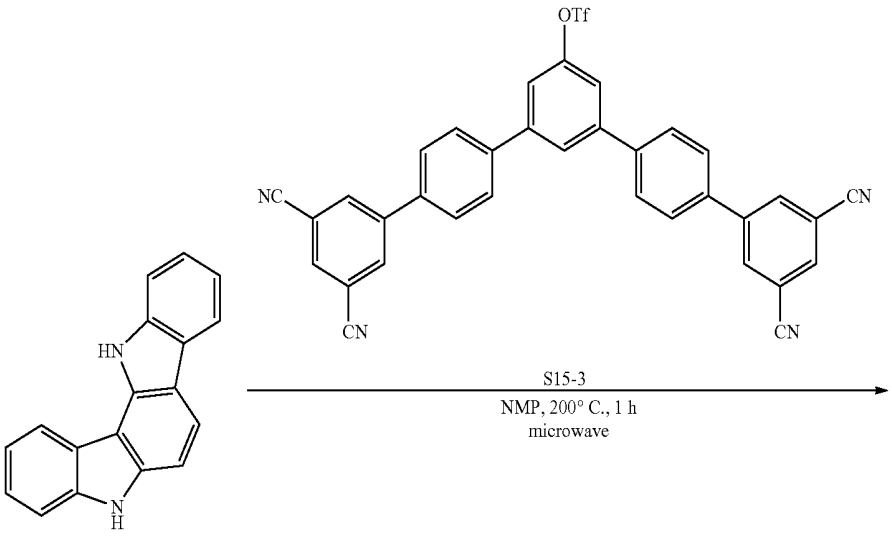
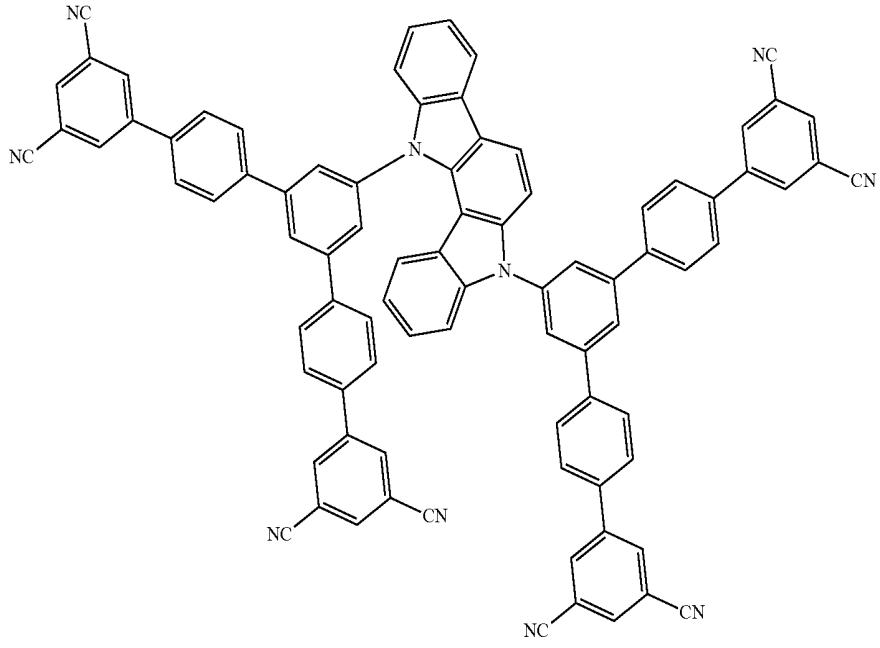
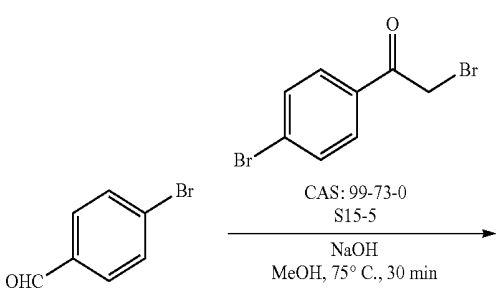


S15-2



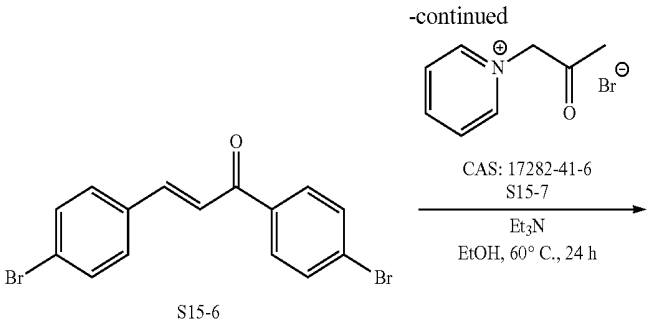
R18

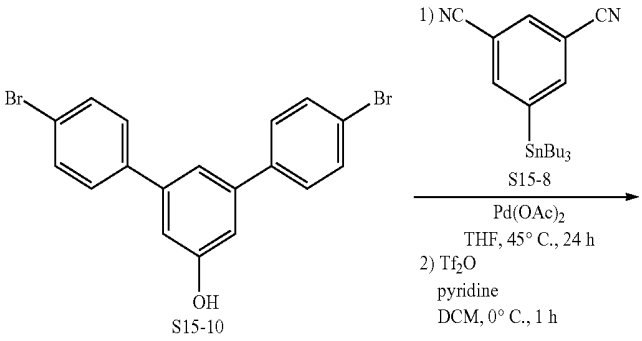
Synthesis of fragment:

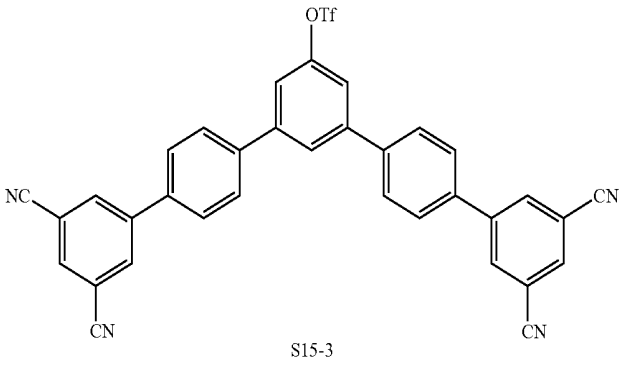


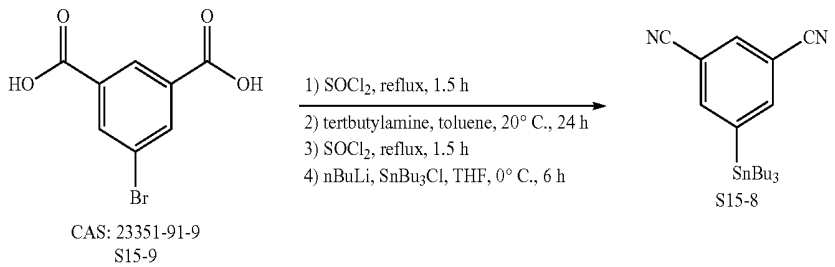
CAS: 1122-91-4
S15-4

-continued


Br
O
Br
S15-6
CAS: 17282-41-6
S15-7
Et_3N
EtOH, 60° C., 24 h


Br
Br
OH
S15-10
1) NC
CN
$SnBu_3$
S15-8
$Pd(OAc)_2$
THF, 45° C., 24 h
2) Tf_2O
pyridine
DCM, 0° C., 1 h

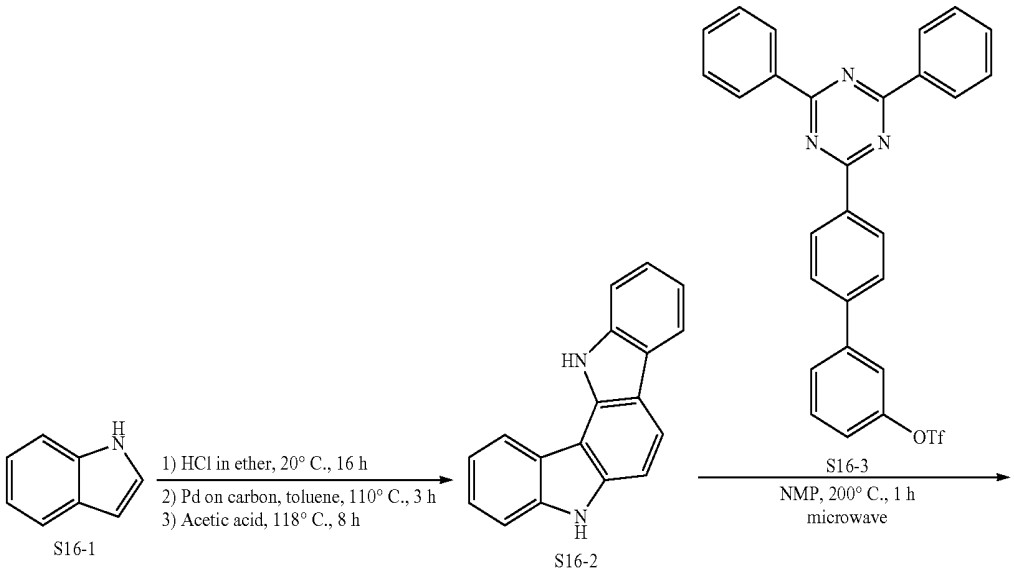

OTf
NC
CN
CN
CN
S15-3

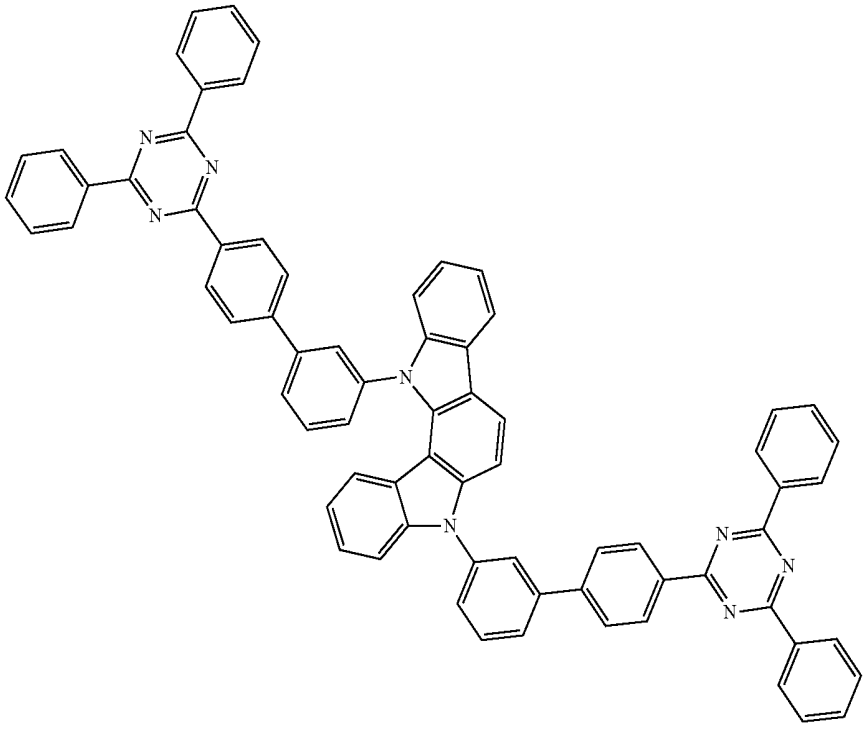

HO
O
O
OH
Br
CAS: 23351-91-9
S15-9
1) $SOCl_2$, reflux, 1.5 h
2) tertbutylamine, toluene, 20° C., 24 h
3) $SOCl_2$, reflux, 1.5 h
4) nBuLi, $SnBu_3Cl$, THF, 0° C., 6 h
NC
CN
$SnBu_3$
S15-8

Compound R108

[0559] Compound R108 may be prepared by a person of ordinary skill following Scheme 16. Starting materials S16-1, S16-4, S16-5, S16-8, and S16-9 are commercially available and may be purchased, for example, from Acros or Aldrich.

Scheme 16

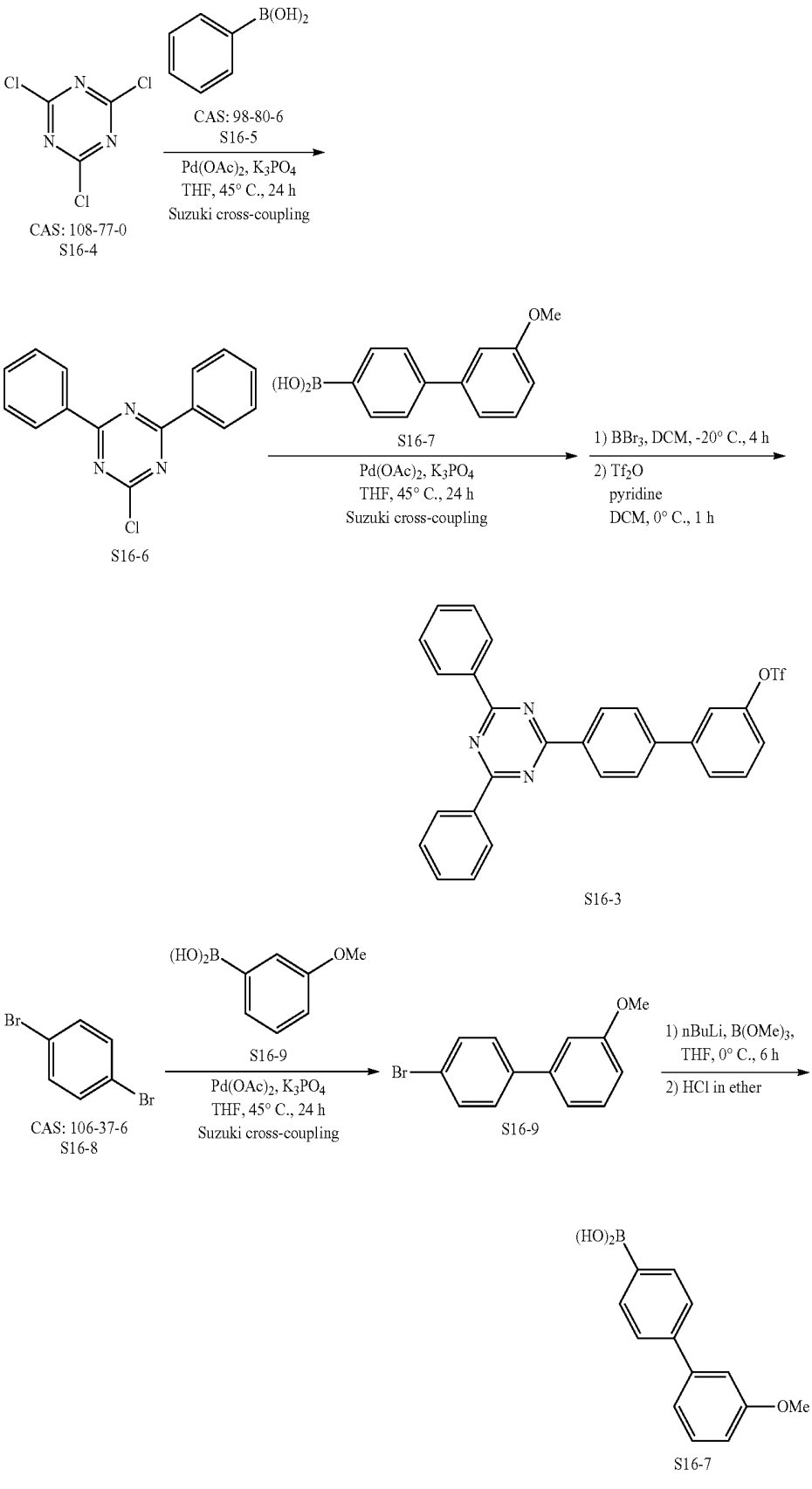




R108

-continued

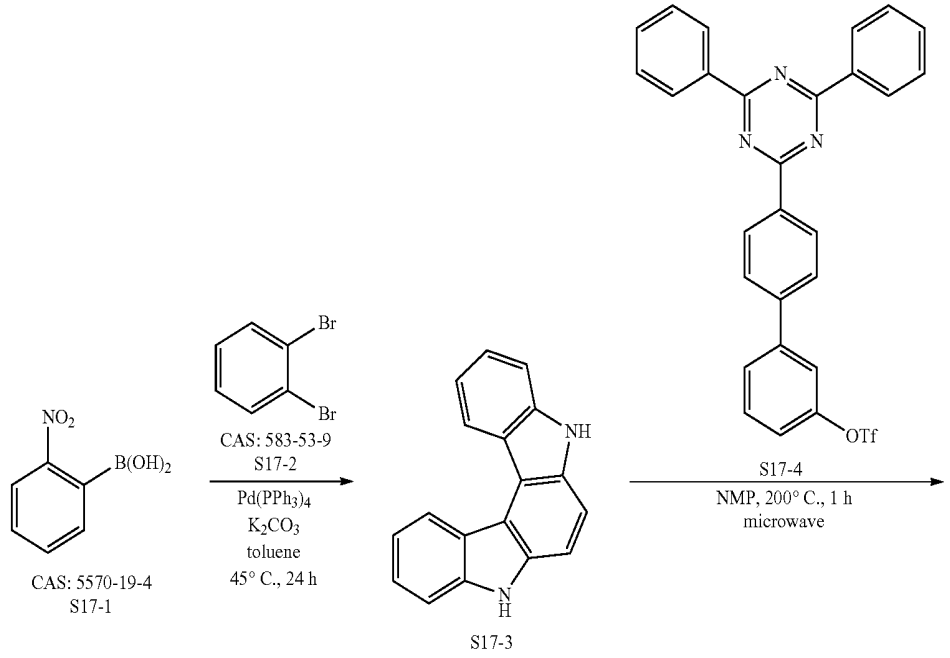
Synthesis of fragment:

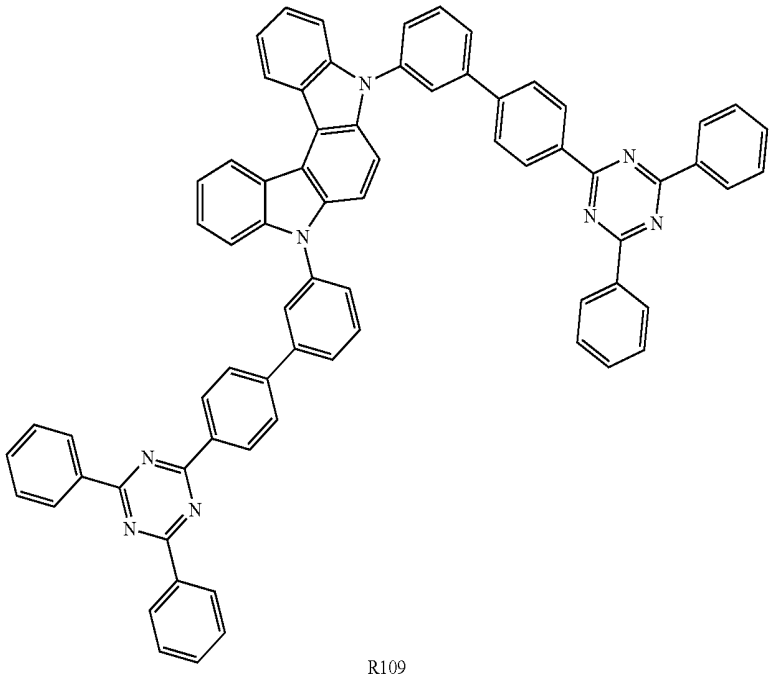


Compound R109

[0560] Compound R109 may be prepared by a person of ordinary skill following Scheme 17. Starting materials S17-1, S17-2, S17-5, S17-6, S17-8, and S17-9 are commercially available and may be purchased, for example, from Acros or Aldrich.

Scheme 17

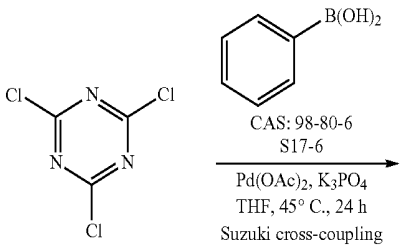




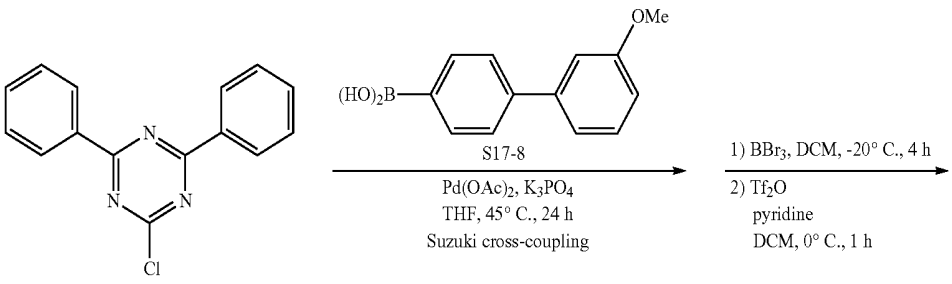
R109

-continued

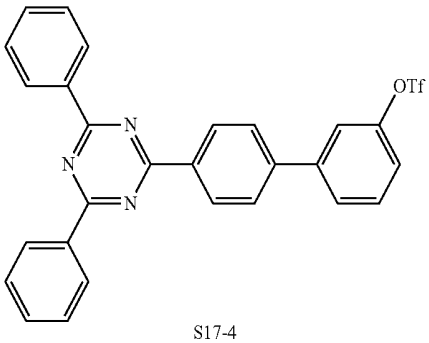
Synthesis of fragment:



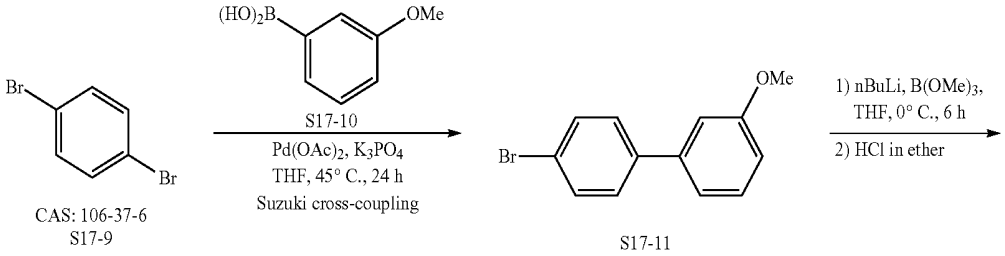
CAS: 108-77-0
S17-5



S17-7

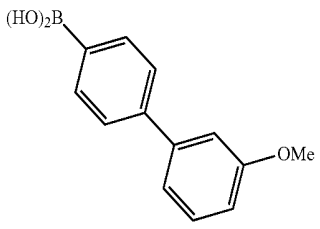


S17-4



CAS: 106-37-6
S17-9

S17-11

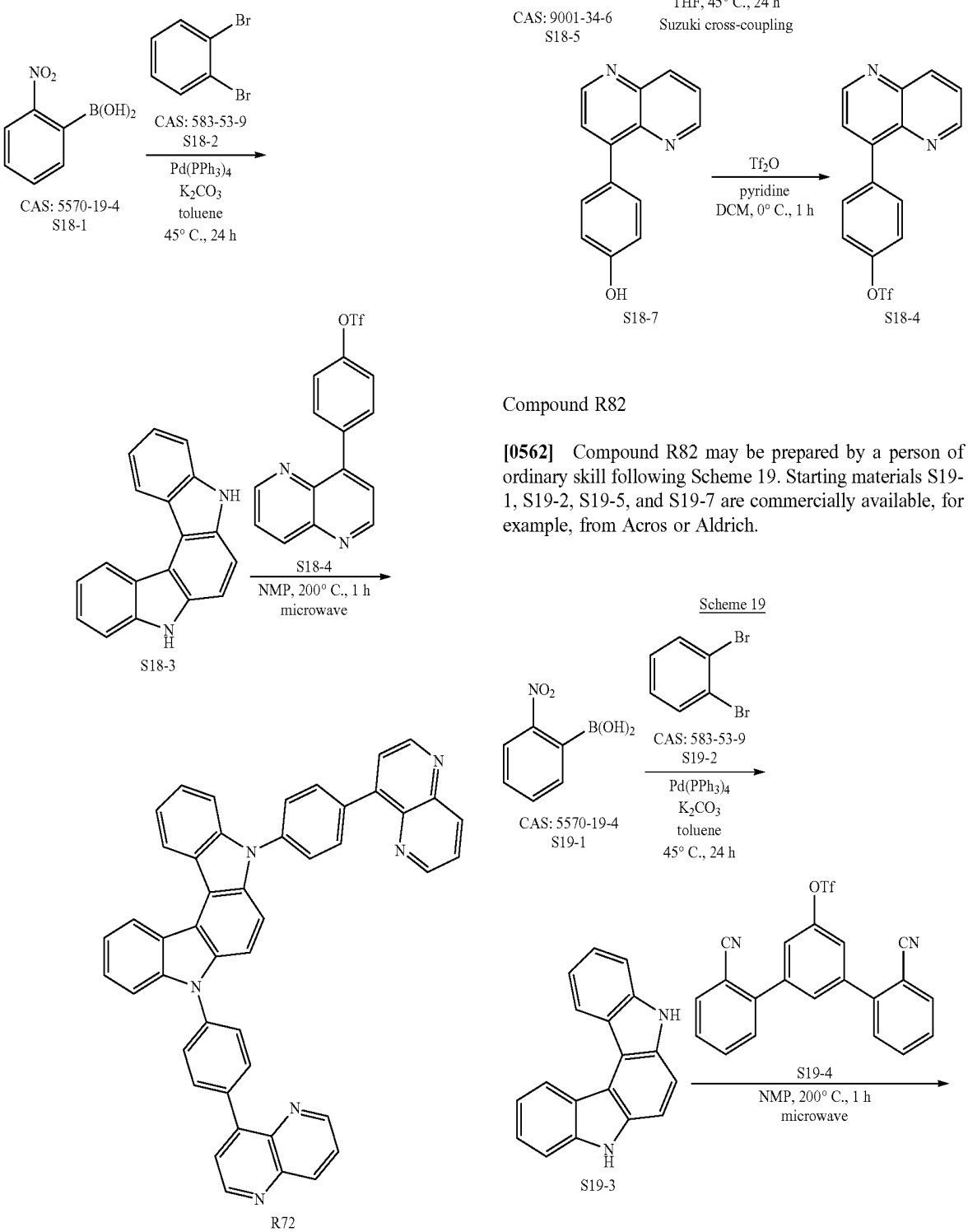


S17-8

Compound R72

[0561] Compound R72 may be prepared by a person of ordinary skill following Scheme 18. Starting materials S18-1, S18-2, S18-5, and S18-6 are commercially available and may be purchased, for example, from Acros, Aldrich, or Bepharm.

Scheme 18



-continued

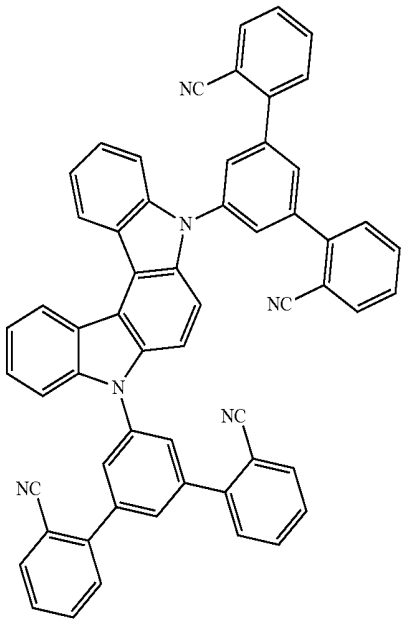
Synthesis of fragment:

Compound R82

[0562] Compound R82 may be prepared by a person of ordinary skill following Scheme 19. Starting materials S19-1, S19-2, S19-5, and S19-7 are commercially available, for example, from Acros or Aldrich.

Scheme 19

-continued

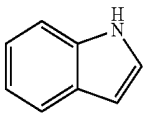


R82

Compound R74

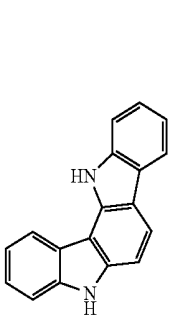
[0563] Compound R74 may be prepared by a person of ordinary skill following Scheme 20. Starting materials S20-1, S20-4, and S20-6 are commercially available and may be purchased, for example, from Acros or Aldrich.

Scheme 20

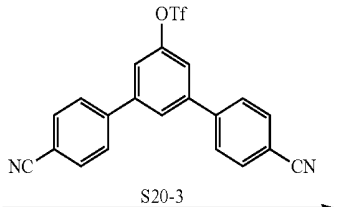


S20-1

1) HCl in ether, 20° C., 16 h
2) Pd on carbon, toluene, 110° C., 3 h
3) Acetic acid, 118° C., 8 h

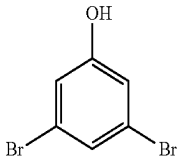


S20-2



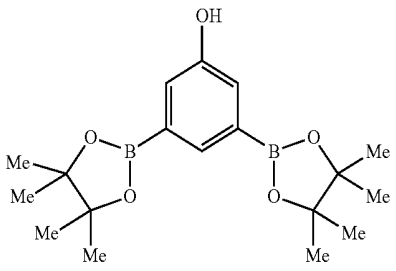
S20-3

NMP, 200° C., 1 h
microwave

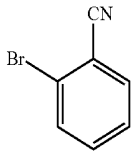


CAS: 626-41-5
S19-5

B_2pin_2
$PdCl_2(PPh_3)_2$
KOAc
dioxane, 80° C., 30 h

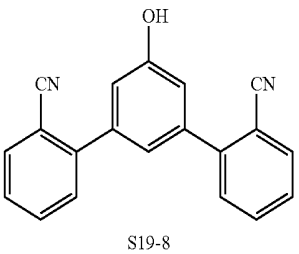


S19-6



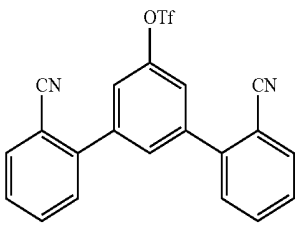
CAS: 2042-37-7
S19-7

$Pd(OAc)_2$, K_3PO_4
THF, 45° C., 24 h
Suzuki
cross-coupling

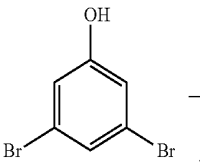


S19-8

Tf_2O
pyridine
DCM, 0° C., 1 h

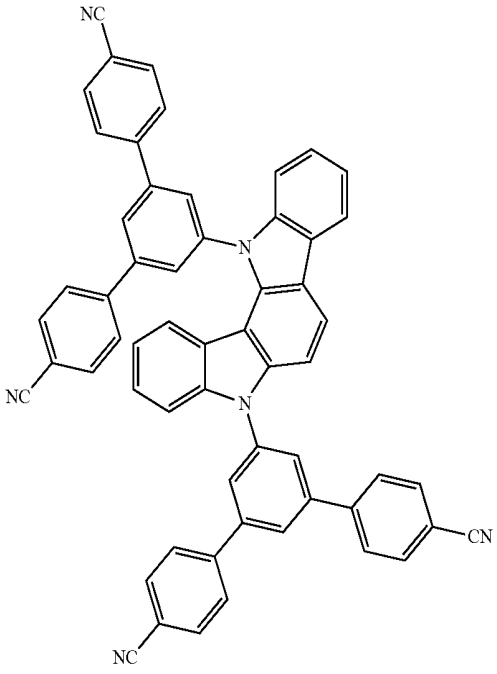


S19-4



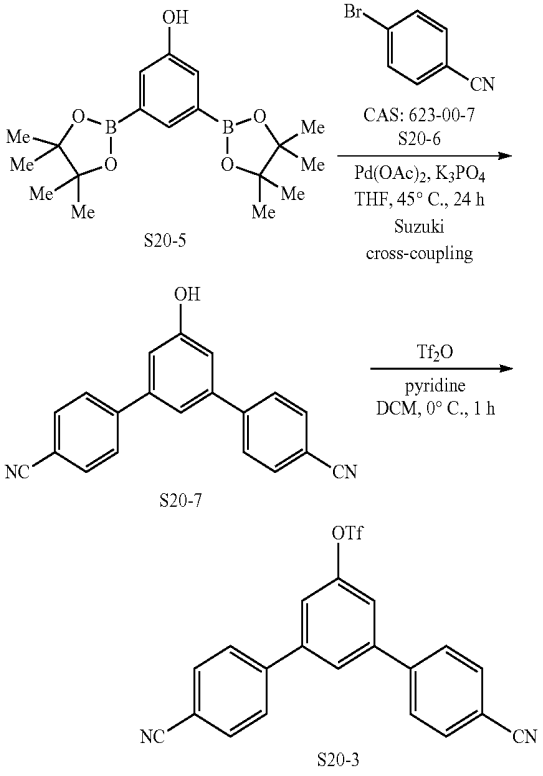
CAS: 626-41-5
S20-5

B_2pin_2
$PdCl_2(PPh_3)_2$
KOAc
dioxane, 80° C., 30 h



R74

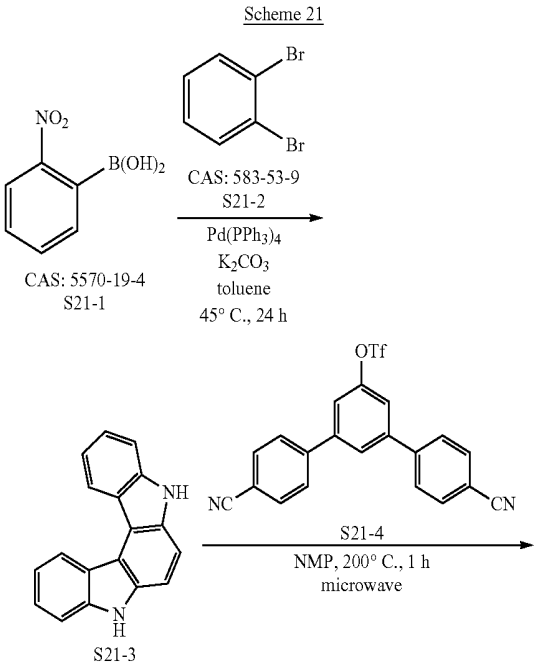
-continued



Compound R57

[0564] Compound R57 may be prepared by a person of ordinary skill following Scheme 21. Starting materials S21-1, S21-2, S21-5, and S21-7 are commercially available, for example, from Acros, Aldrich, or Alfa-Aesar.

Scheme 21



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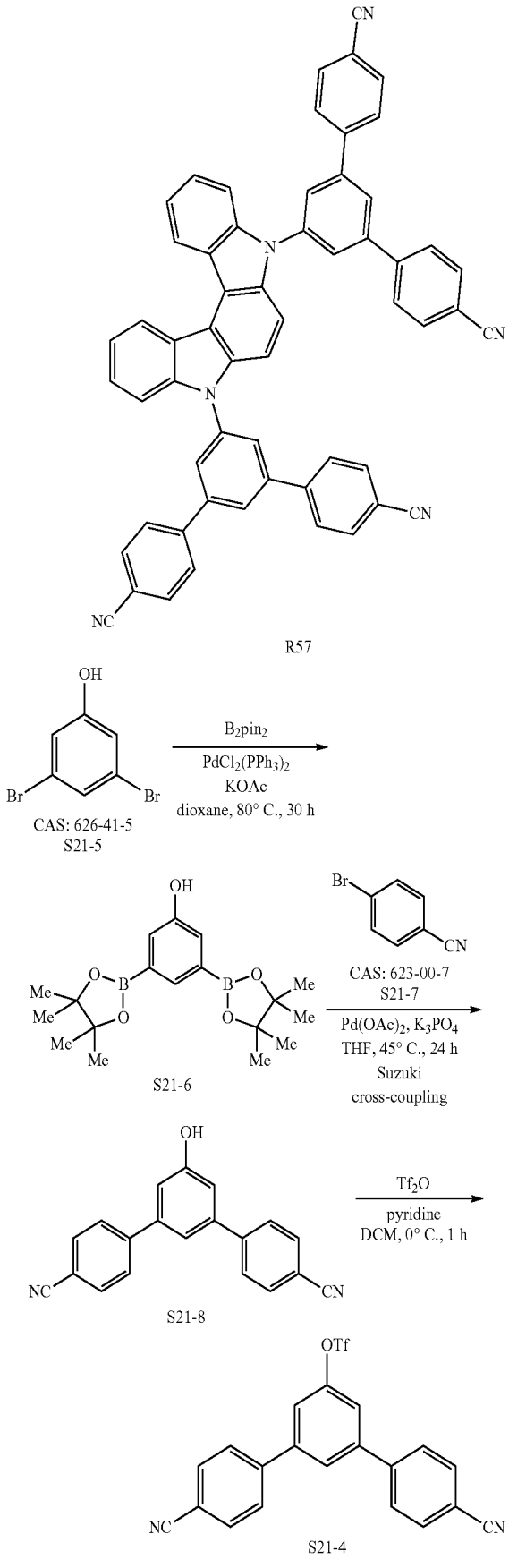
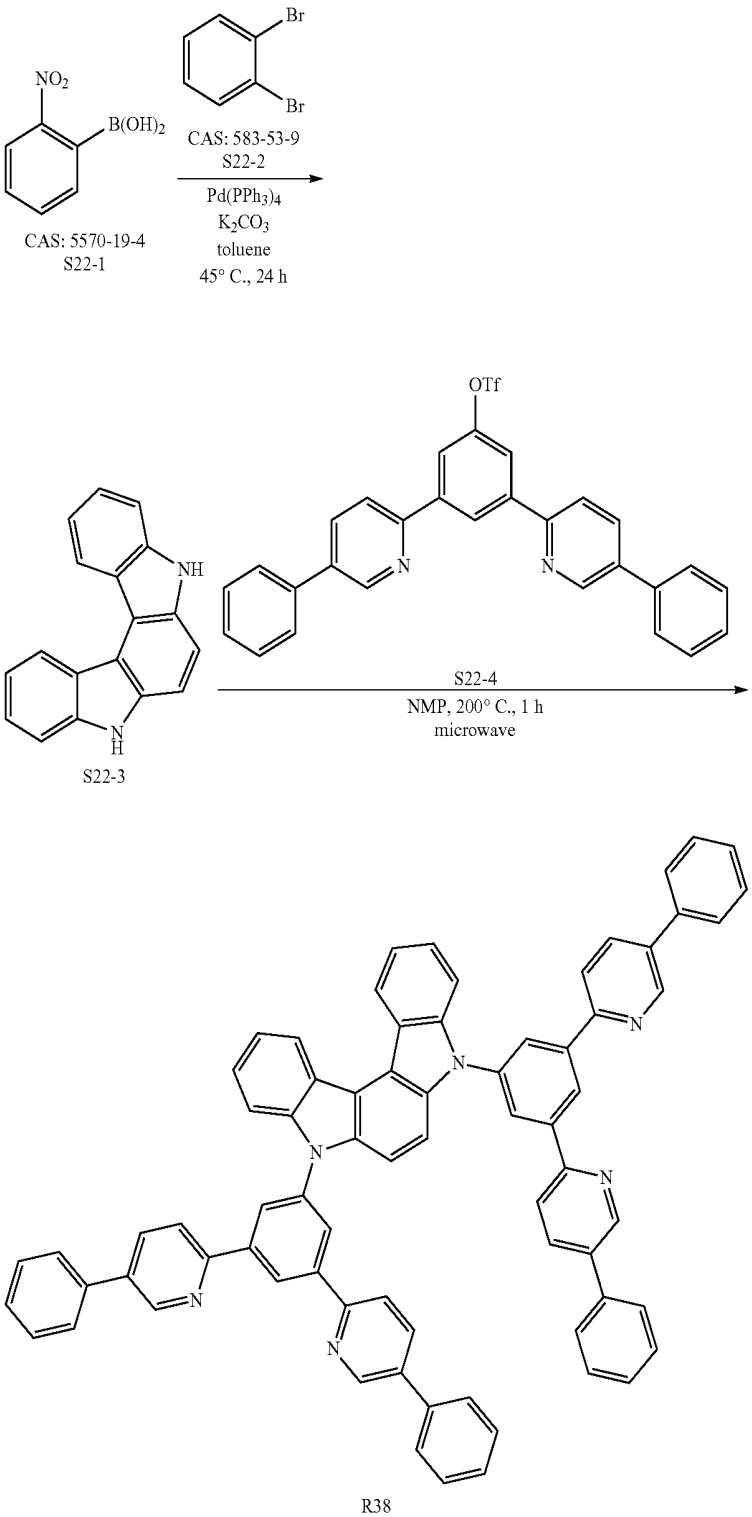


Compound R38

[0565] Compound R38 may be prepared by a person of ordinary skill following Scheme 22. Starting materials S22-1, S22-2, S22-5, and S22-7 are commercially available, for example, from Acros, Arkpharm, or Aldrich.

Scheme 22



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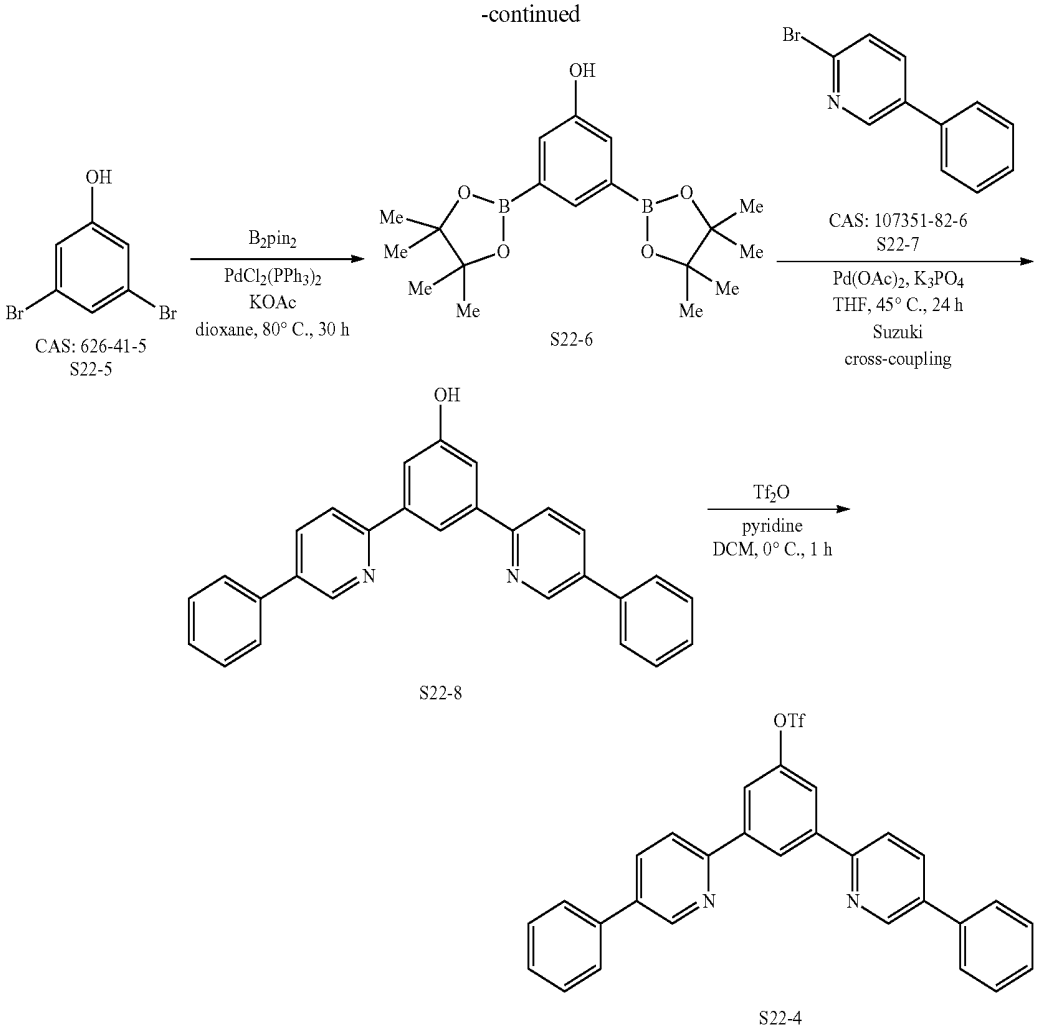
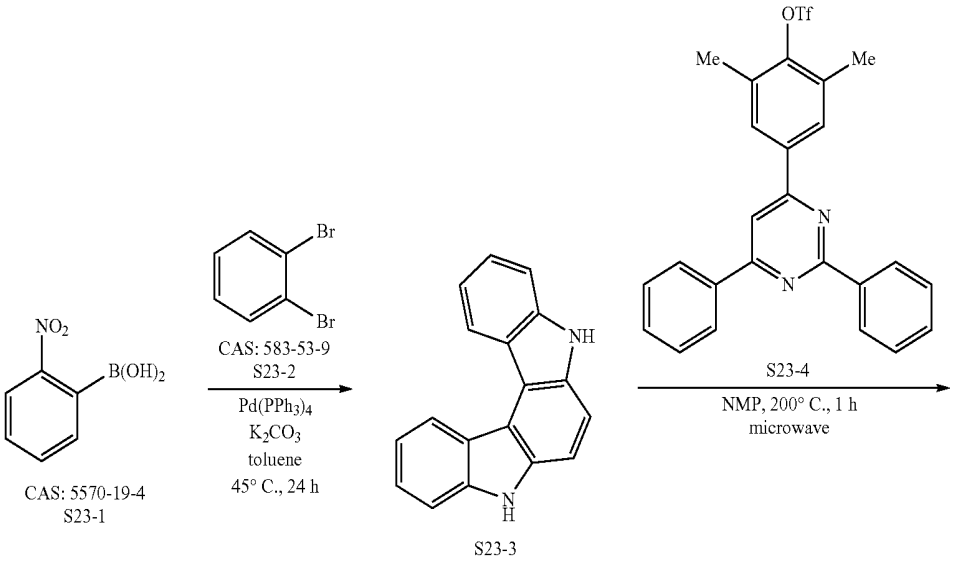


Compound R50

[0566] Compound R50 may be prepared by a person of ordinary skill following Scheme 23. Starting materials S23-1, S23-2, S23-5, and S23-6 are commercially available, for example, from Acros, TCI America, or Aldrich.

Scheme 23



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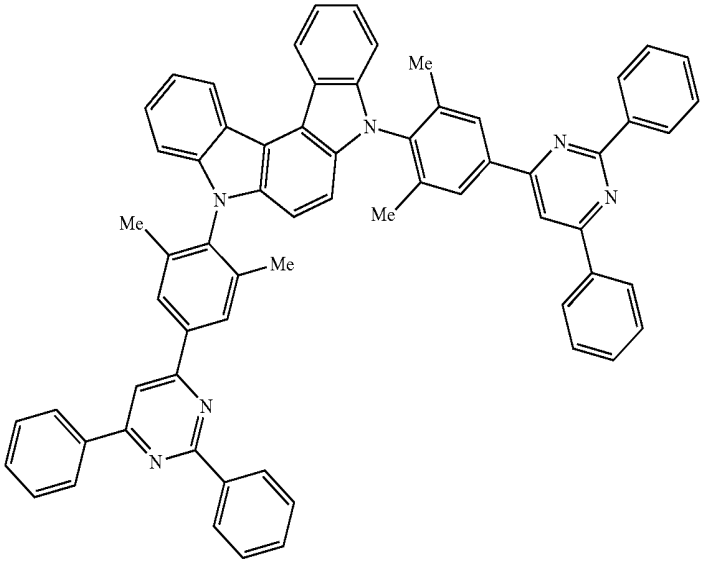
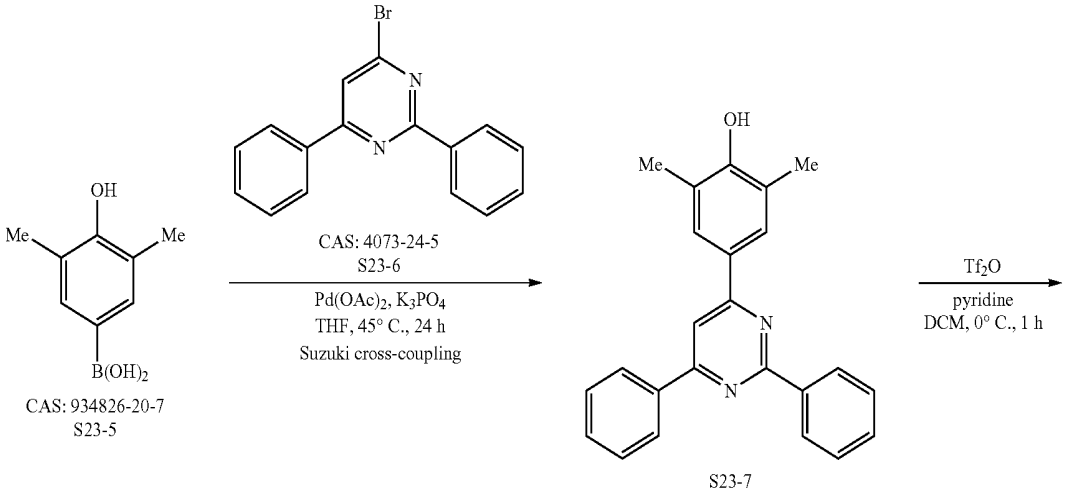
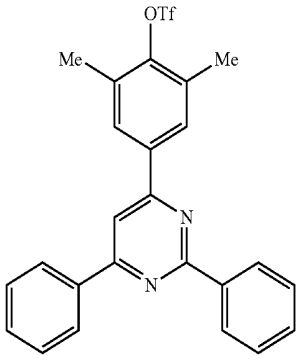


R50

Synthesis of fragment:



-continued

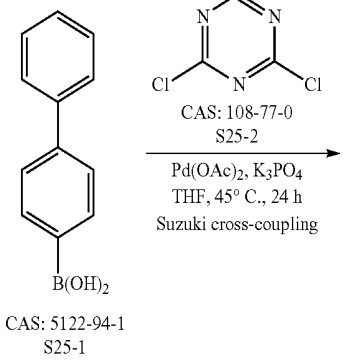


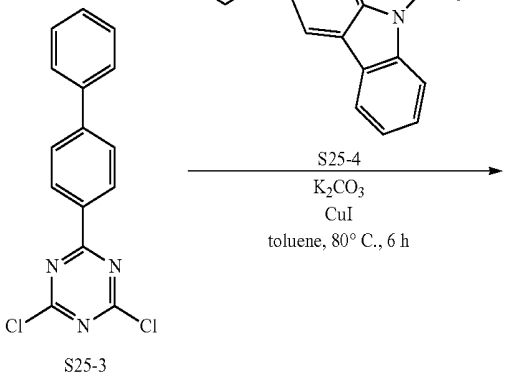
S23-4

Compound R110

[0567] Compound R110 may be prepared by a person of ordinary skill following Scheme 24. Starting materials S25-1, S25-2, S25-5 and S25-6 are commercially available, for example, from Acros or Aldrich.

Scheme 24





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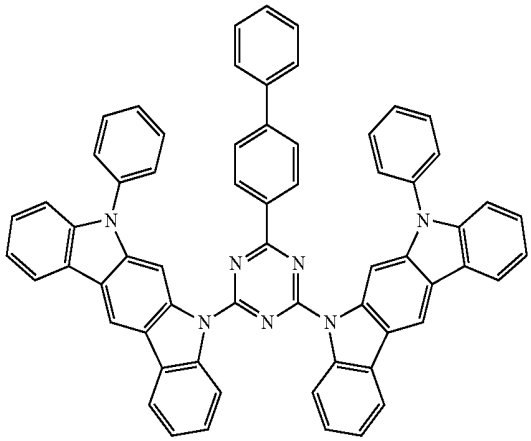
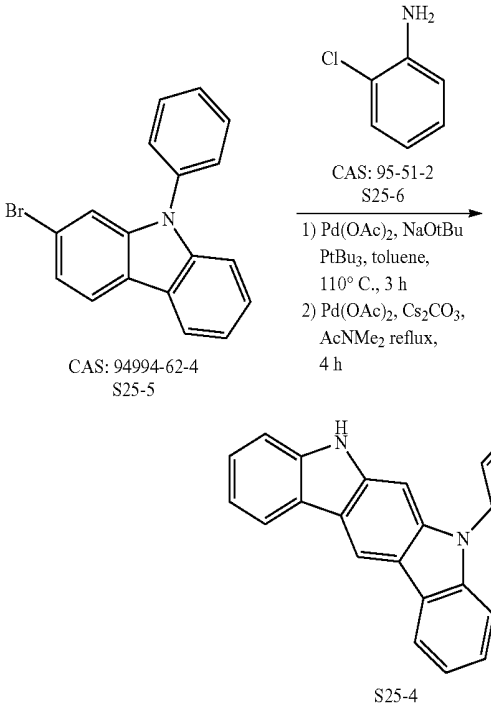


R110

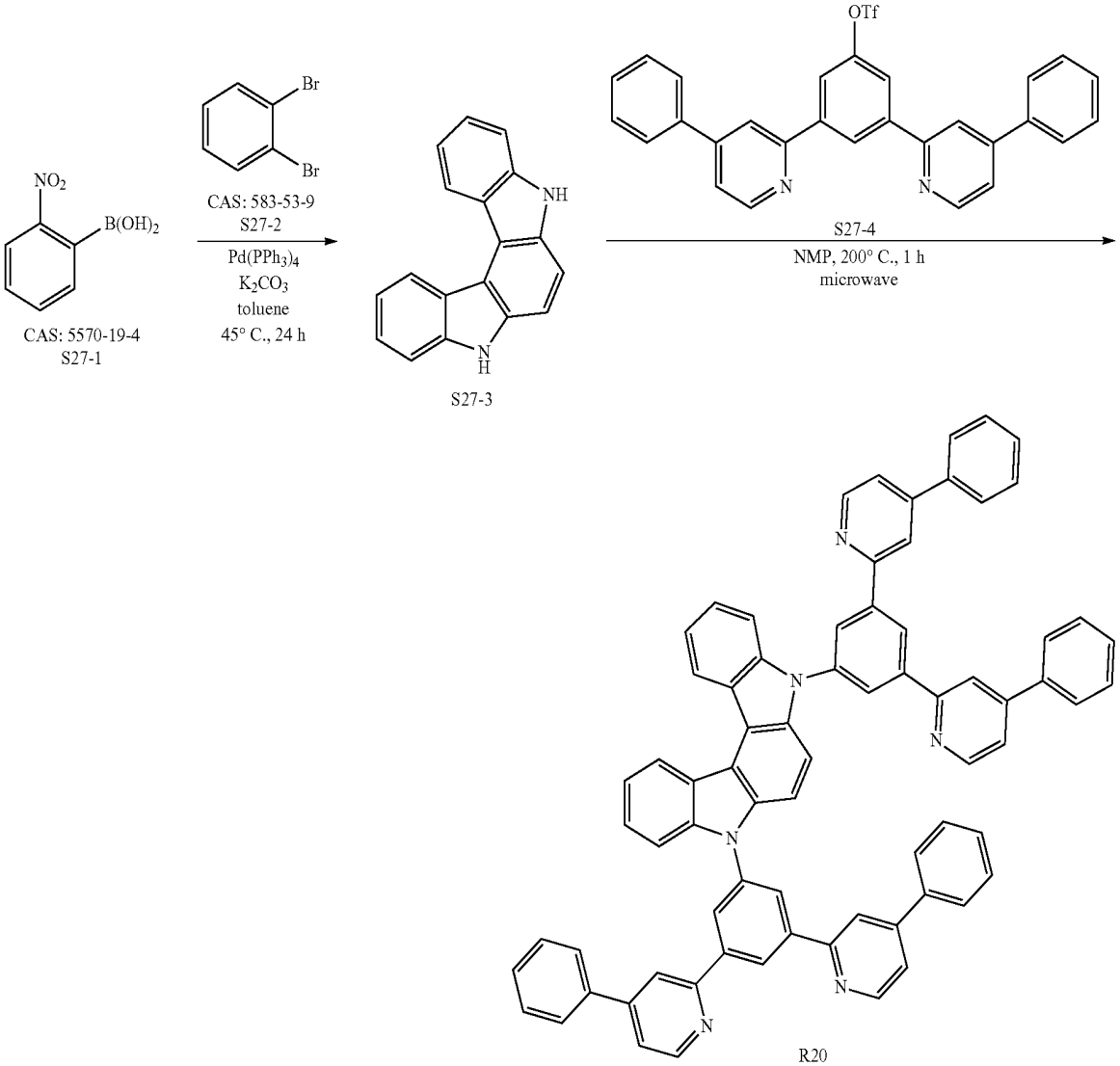
Synthesis of fragment:



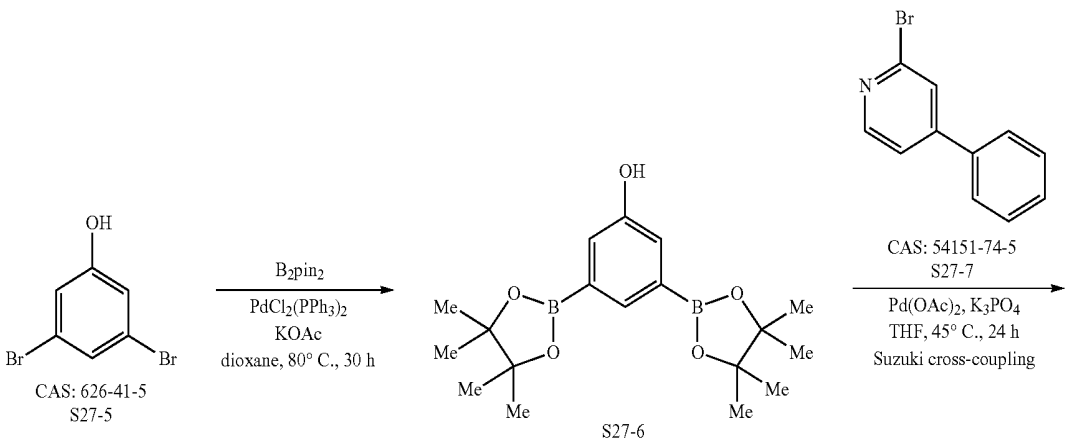
Compound R20

[0568] Compound R20 may be prepared by a person of ordinary skill following Scheme 25. Starting materials S27-1, S27-2, S27-5, and S27-7 are commercially available, for example, from Acros, Arkpharm, or Aldrich.

Scheme 25



Synthesis of fragment:



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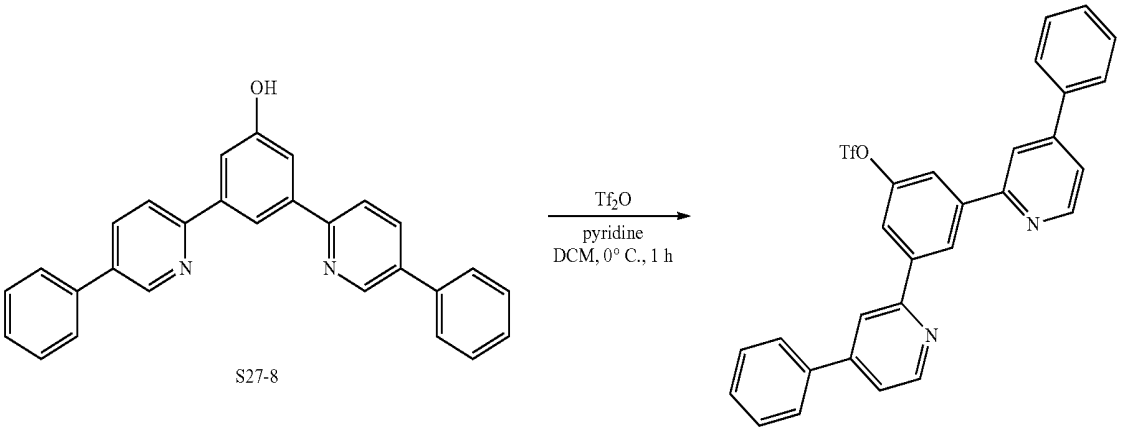
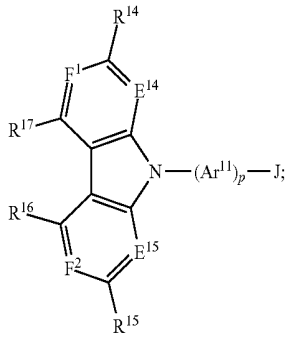


[0569] The teachings of all patents, published applications and references cited herein are incorporated by reference in their entirety.

[0570] While this invention has been particularly shown and described with references to example embodiments thereof, it will be understood by those skilled in the art that various changes in form and details may be made therein without departing from the scope of the invention encompassed by the appended claims.

1. A molecule represented by structural formula (I):

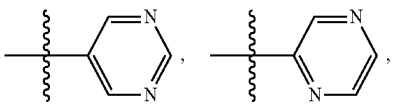


(I)

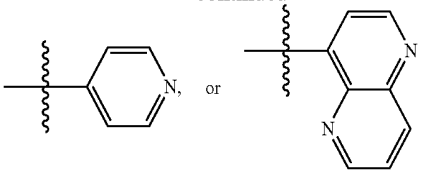
wherein:

E^{14}, and E^{15} are, each independently, CR^A or N, wherein R^A, for each occurrence independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

J is any moiety selected from —CN,



-continued



and is optionally substituted with one or more R^{11}, each independently selected from C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

F^1 is C—$(Ar^{12})_q$-G;

F^2 is CR^B or N, wherein R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN, or —$(Ar^{12})_q$-G;

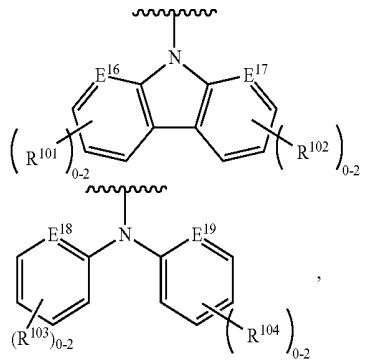
Ar^{11}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

Ar^{12}, for each occurrence independently, is phenyl optionally substituted with one to four C_1-C_6 alkyls;

p is 0, 1, or 2;

q is 0 or 1; and

G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



or

wherein:

E^{16}, E^{17}, E^{18}, and E^{19} are, each independently, CR^C or N, wherein R^C is H, a C_1-C_3 alkyl, halo, or —CN; and

R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a C_6-C_{18} aryl, a 5-20 atom heteroaryl, a halo, or —CN;

provided that the molecule is not represented by any structural formula in Table NN1.

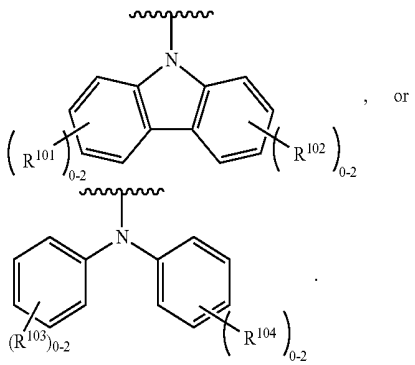
2. The molecule of claim **1**, wherein J is unsubstituted.

3. The molecule of claim **1**, wherein J is substituted with one or more R^{11} selected from C_1-C_6 alkyl or C_6-C_{18} aryl.

4. The molecule of claim **3**, wherein J is substituted with one or more R^{11} selected from C_1-C_6 alkyl or phenyl.

5. The molecule of claim **1**, wherein F^2 is CR^B.

6. The molecule of claim **1**, wherein G, for each occurrence independently, is a moiety represented by one of the following structural formulas:



, or

.

7. The molecule of claim **1** any one of the preceding claims, wherein:

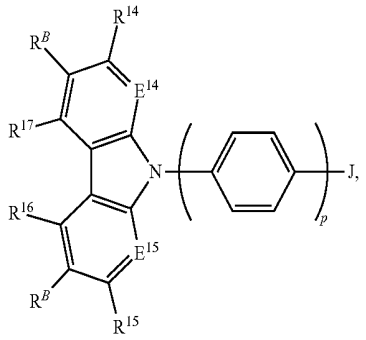
R^A, for each occurrence independently, is H or a C_1-C_6 alkyl;

R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, or a C_3-C_6 cycloalkyl; and

F^2 is CR^B; and

R^B is H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or $—(Ar^{12})_q$-G.

8. The molecule of claim **1**, represented by the following structural formula:



wherein:

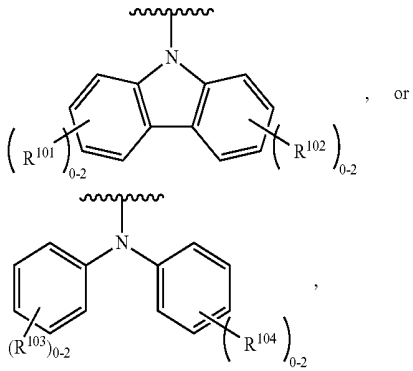
E^{14}, and E^{15}, are, each independently, CR^A or N, wherein R^A, for each occurrence independently, is H or a C_1-C_6 alkyl;

p is 0 or 1;

R^H is a C_6-C_{18} aryl or a 5-20 atom heteroaryl;

R^{14}, R^{15}, R^{16}, and R^{17} are, each independently, H, a C_1-C_6 alkyl, a C_3-C_{18} cycloalkyl, a halo, or —CN;

R^B is, for each occurrence independently, H, a C_1-C_6 alkyl, a C_3-C_6 cycloalkyl, or a moiety represented by one of the following structural formulas:



, or

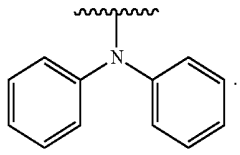
,

wherein:

R^{101}, R^{102}, R^{103}, and R^{104} are, each independently, a C_1-C_6 alkyl or a C_3-C_6 cycloalkyl.

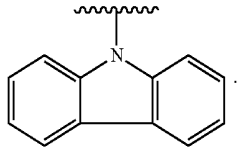
9. The molecule of claim **1**, wherein E^{14} and E^{15} are CR^A.

10. The molecule of claim **1**, wherein R^B is, for each occurrence independently, H or a moiety represented by the following structural formula:



.

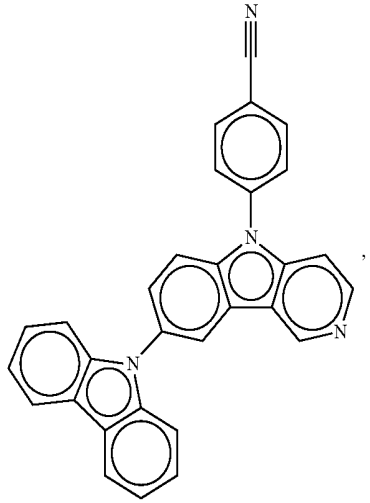
11. The molecule of claim **1**, wherein R^B is, for each occurrence independently, H or a moiety represented by the following structural formula:



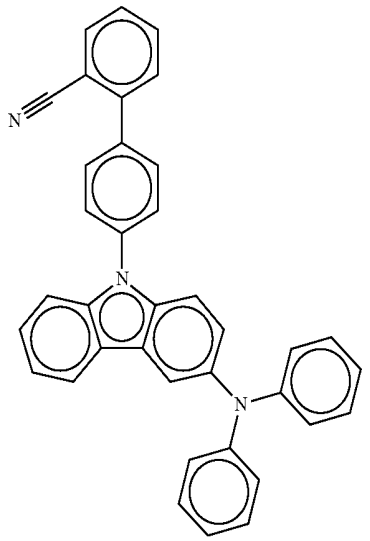
.

12. The molecule of claim **1**, wherein J is —CN.

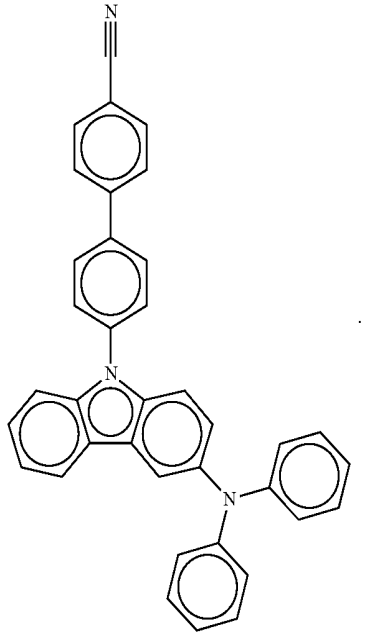
13. The molecule of claim **12**, wherein the molecule is represented by one of the following structural formulas:



,

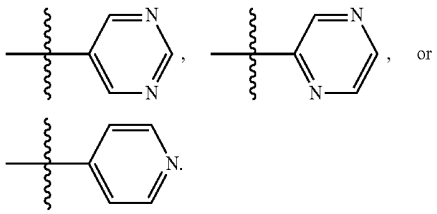


, or



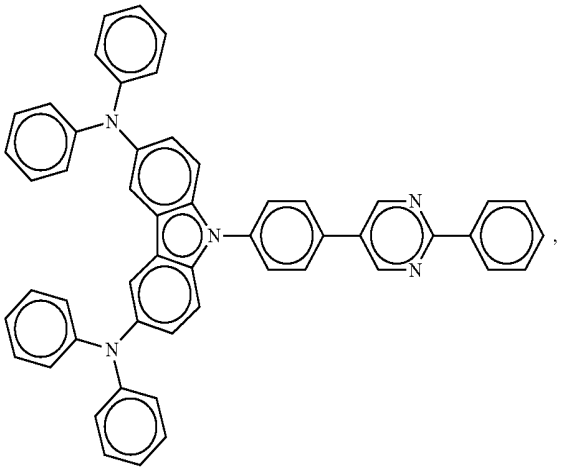
.

14. The molecule of claim **1**, wherein J is

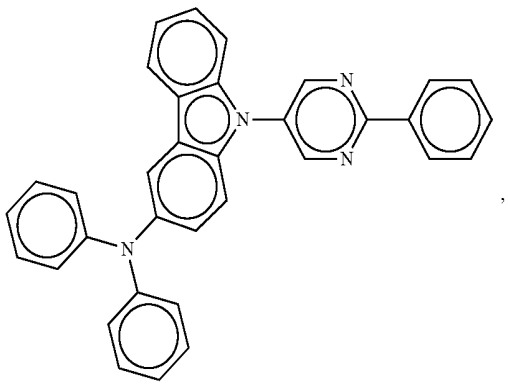


, , or

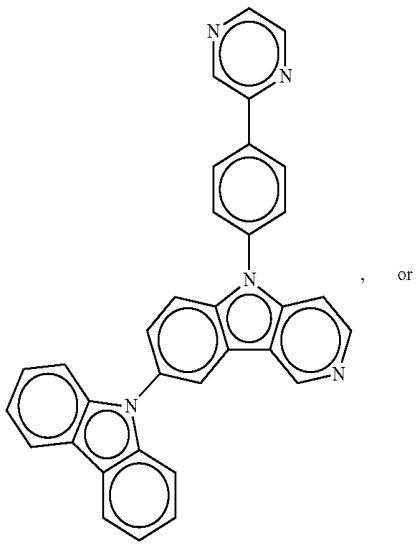
15. The molecule of claim **14**, wherein the molecule is represented by one of the following structural formulas:



,

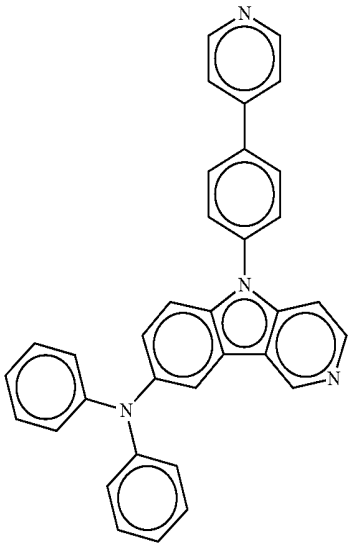


,

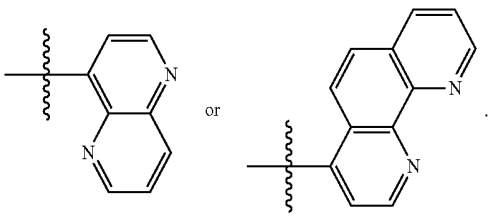


, or

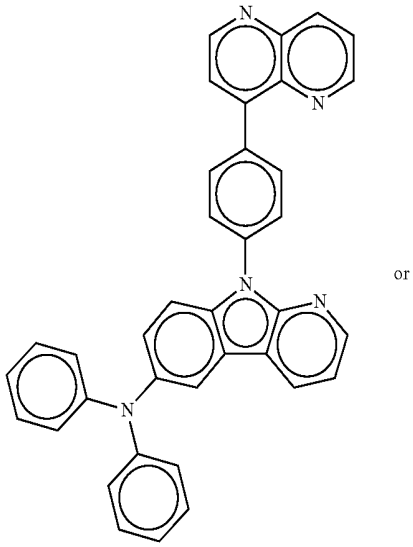
-continued



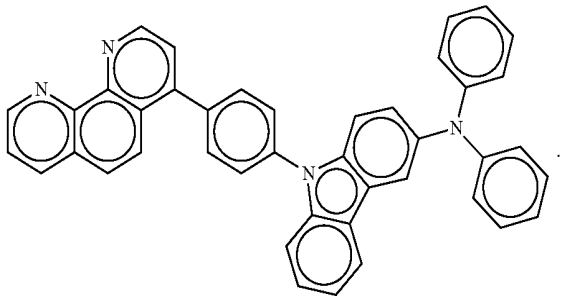
16. The molecule of claim **1**, wherein J is



17. The molecule of claim **16**, wherein the molecule is represented by one of the following structural formulas:



or



18-127. (canceled)

128. An organic light-emitting device containing:

a first electrode;

a second electrode; and

an organic layer disposed between the first electrode and the second electrode, wherein the organic layer comprises at least one molecule as defined by claim **1**.

* * * * *

专利名称(译)	有机发光二极管材料		
公开(公告)号	US20180212158A1	公开(公告)日	2018-07-26
申请号	US15/744571	申请日	2016-07-13
[标]申请(专利权)人(译)	哈佛大学校长及研究员协会		
申请(专利权)人(译)	主席和哈佛学院院士		
当前申请(专利权)人(译)	主席和哈佛学院院士		
[标]发明人	ASPURU GUZIK ALAN GOMEZ BOMBARELLI RAFAEL HIRZEL TIMOTHY D AGUILERA IPARRAGUIRRE JORGE		
发明人	ASPURU-GUZIK, ALAN GOMEZ-BOMBARELLI, RAFAEL HIRZEL, TIMOTHY D. AGUILERA-IPARRAGUIRRE, JORGE		
IPC分类号	H01L51/00 C07D471/04 C09K11/06 C07D209/88 C07D519/00 C07D417/04 C07D403/14 C07D487/04		
CPC分类号	H01L51/0072 C07D471/04 C09K11/06 H01L51/0067 H01L51/0061 C07D209/88 C07D519/00 C07D417/04 C07D403/14 C07D487/04 C09K2211/1018 H01L51/5012 H01L51/0071 C09K2211/1022		
优先权	62/239556 2015-10-09 US 62/191766 2015-07-13 US 62/208190 2015-08-21 US 62/277316 2016-01-11 US		
外部链接	USPTO		

摘要(译)

描述的hein是用于有机发光二极管的分子。实例分子包含至少一个受体部分A，至少一个供体部分D和任选的一个或多个桥部分B.每个部分A共价连接至部分B或部分D，每个部分D共价连接至任一部分。 M部分或部分A和每个B共价连接至至少一个部分A和至少一个部分D.本文定义了部分A，D和B的值和优选值。