Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Enhancement of Intramolecular Charge Transfer Strength in Diphenylamine Substituted Symmetric 1,3,4-Oxadiazole Derivatives

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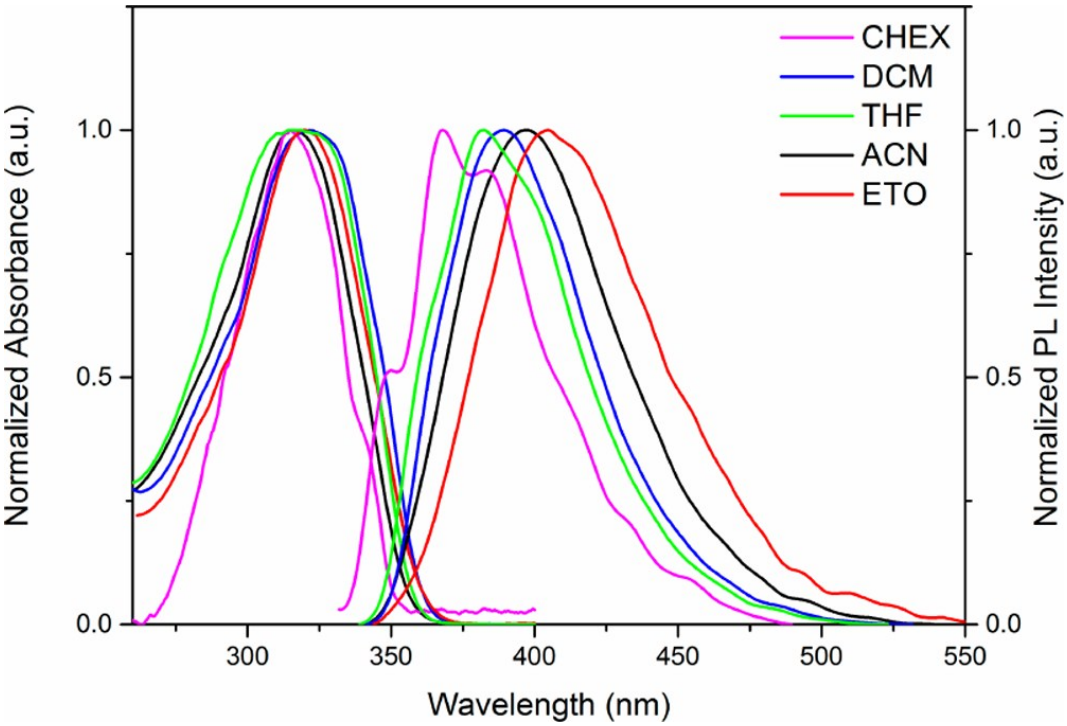

Figure S1 Normalized UV−vis absorption and fluorescence emission spectra of BOXD-*p*-OCH_3

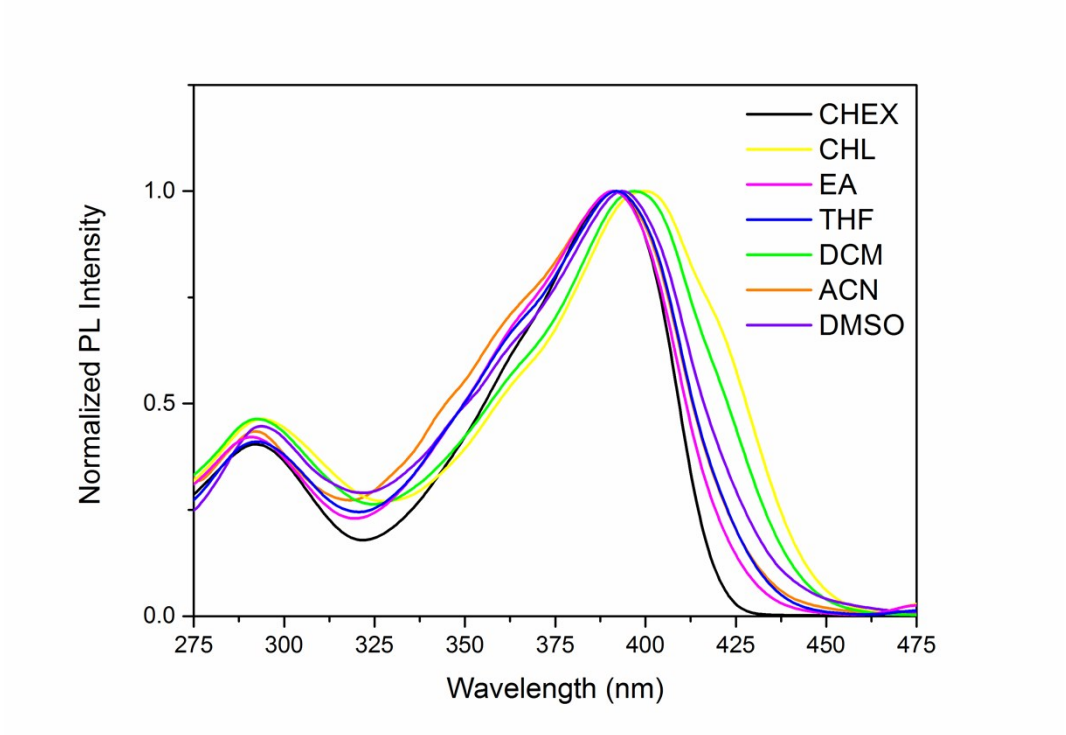

Figure S2 Normalized excitation spectra of DPAOXD

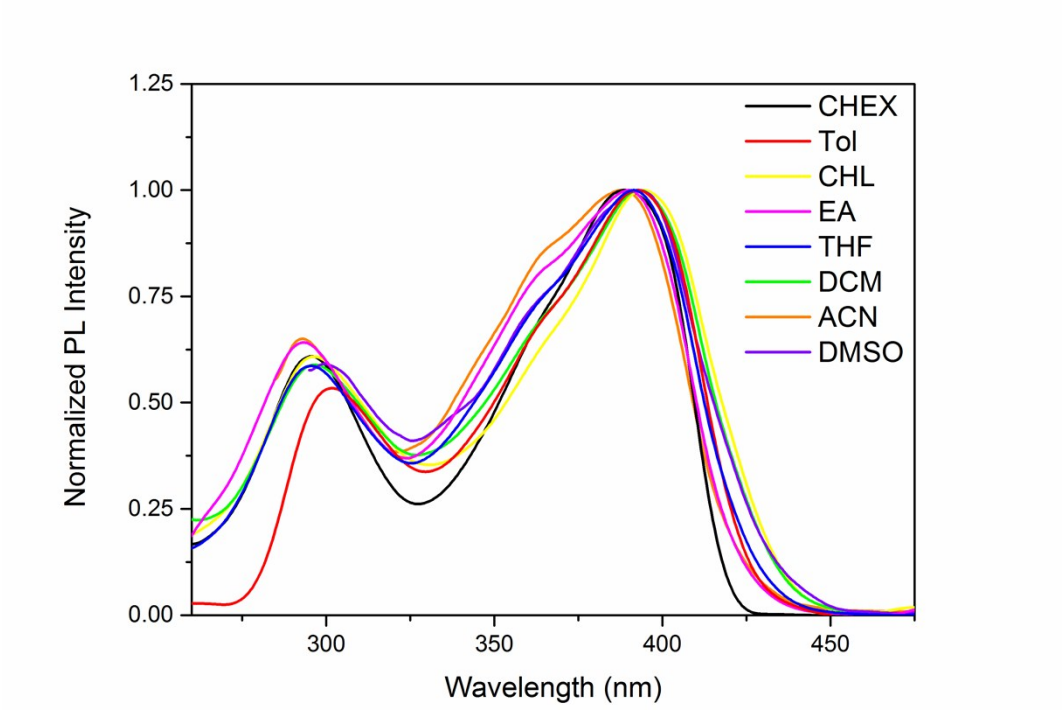

Figure S3 Normalized excitation spectra of DPAOXDBEN

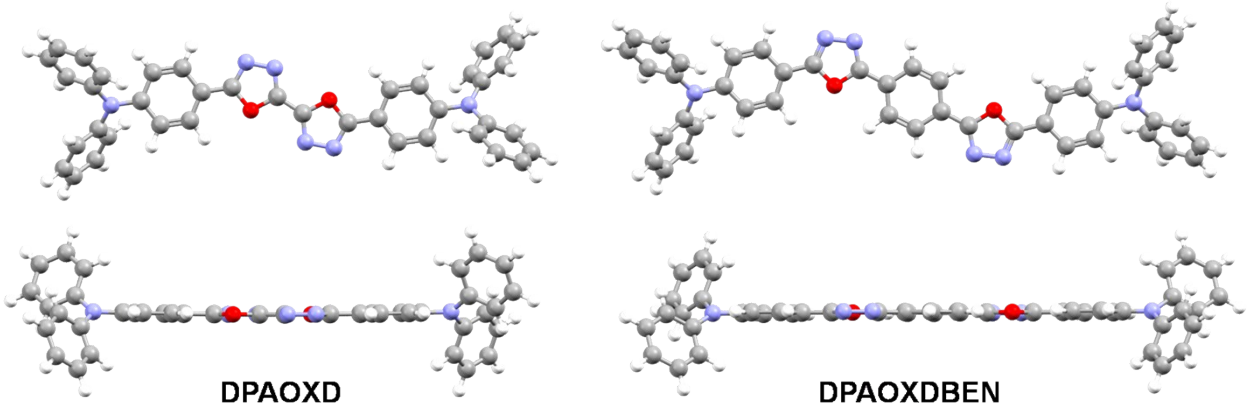

Figure S6 Optimized molecular structures in the first excited state of DPAOXD and DPAOXDBEN

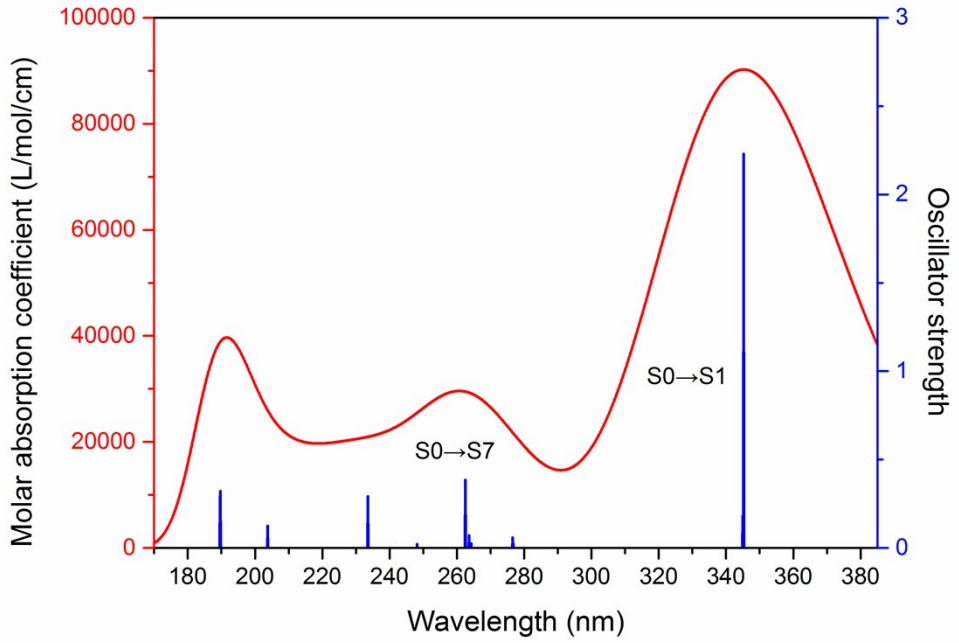

Figure S4 Calculated absorption spectrum of DPAOXD in CHEX

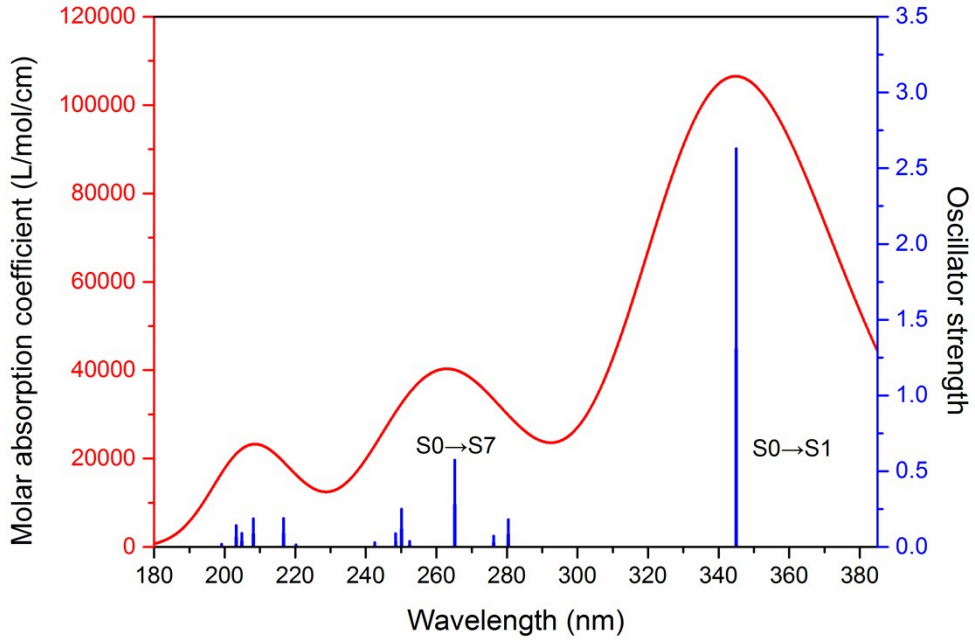

Figure S5 Calculated absorption spectrum of DPAOXDBEN in CHEX

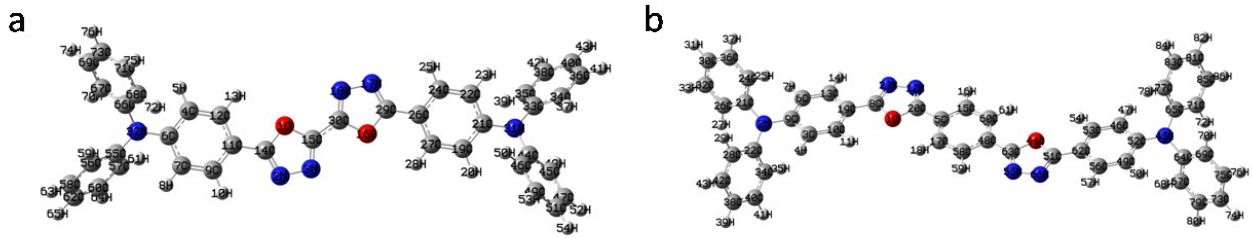

Figure S7 Molecular structure of (a) DPAOXD and (b) DPAOXDBEN

Table S1 Calculated bond length of optimized structure of DPAOXD in the ground state and first excited state

Bond		S_0	S_1	variation
O1	C14	1.3585	1.3659	0.0074
O1	C15	1.3512	1.364	0.0128
N2	N3	1.3804	1.3388	-0.0416
N2	C14	1.2978	1.3239	0.0261
N3	C15	1.2909	1.328	0.0371
C4	C6	1.402	1.4098	0.0078
C4	C12	1.3828	1.3747	-0.0081
C6	C7	1.4036	1.4126	0.009
C6	N32	1.4027	1.3999	-0.0028
C7	C9	1.3809	1.372	-0.0089
C9	C11	1.3977	1.4144	0.0167
C11	C12	1.3962	1.4128	0.0166
C11	C14	1.4513	1.4201	-0.0312
C15	C30	1.4445	1.4034	-0.0411
C55	C56	1.3955	1.3982	0.0027
C55	C57	1.3961	1.3983	0.0022
C56	C58	1.3884	1.3869	-0.0015
C57	C60	1.3883	1.3871	-0.0012
C58	C62	1.3902	1.3913	0.0011
C60	C62	1.3907	1.391	0.0003
C66	C67	1.3954	1.3981	0.0027
C66	C68	1.3961	1.3983	0.0022
C67	C69	1.3885	1.3869	-0.0016
C68	C71	1.3883	1.3872	-0.0011
C69	C73	1.3903	1.3914	0.0011
C71	C73	1.3905	1.391	0.0005

Table S2 Calculated angles of optimized structure of DPAOXD in the ground state and first excited state

	angle		S0	S1	variation
C14	O1	C15	102.39	102.38	-0.01
N3	N2	C14	106.81	107.87	1.06
N2	N3	C15	106.01	106.72	0.71
C6	C4	C12	120.66	120.69	0.03
C4	C6	C7	118.54	118.74	0.2
C4	C6	N32	120.74	120.68	-0.06
C7	C6	N32	120.72	120.58	-0.14
C6	C7	H8	119.56	119.3	-0.26
C6	C7	C9	120.66	120.67	0.01
C7	C9	C11	120.54	120.67	0.13
C9	C11	C12	119.08	118.61	-0.47
C9	C11	C14	119.55	120.02	0.47
C12	C11	C14	121.37	121.37	0
C4	C12	C11	120.53	120.62	0.09
O1	C14	N2	111.83	111.22	-0.61
O1	C14	C11	119.33	120.44	1.11
N2	C14	C11	128.84	128.34	-0.5
O1	C15	N3	112.96	111.8	-1.16
O1	C15	C30	118.64	119.85	1.21
N3	C15	C30	128.4	128.35	-0.05
C6	N32	C55	120.77	120.27	-0.5
C6	N32	C66	120.76	120.37	-0.39
C55	N32	C66	118.47	119.35	0.88
N32	C55	C56	120.04	120.29	0.25
N32	C55	C57	120.58	120.26	-0.32
C56	C55	C57	119.37	119.45	0.08
C55	C56	C58	120.15	120.02	-0.13
C55	C57	C60	120.12	120.03	-0.09
C56	C58	C62	120.46	120.53	0.07
C57	C60	C62	120.46	120.51	0.05
C58	C62	C60	119.43	119.46	0.03
N32	C66	C67	120.05	120.27	0.22
N32	C66	C68	120.58	120.27	-0.31
C67	C66	C68	119.37	119.46	0.09
C66	C67	C69	120.15	120.03	-0.12
C66	C68	C71	120.12	120.02	-0.1
C67	C69	C73	120.44	120.52	0.08
C68	C71	C73	120.46	120.52	0.06
C69	C73	C71	119.44	119.46	0.02

Table S3 Calculated torsions of optimized structure of DPAOXD in the ground state and first excited state

Torsion				S_0	S_1	variation
C15	O1	C14	N2	-0.04	0.14	0.18
C15	O1	C14	C11	179.86	-179.56	-359.42
C14	O1	C15	N3	0	-0.15	-0.15
C14	O1	C15	C30	-179.76	179.58	359.34
C14	N2	N3	C15	-0.06	-0.01	0.05
N3	N2	C14	O1	0.06	-0.09	-0.15
N3	N2	C14	C11	-179.83	179.58	359.41
N2	N3	C15	O1	0.03	0.1	0.07
N2	N3	C15	C30	179.76	-179.6	-359.36
C12	C4	C6	C7	-0.34	0.12	0.46
C12	C4	C6	N32	179.57	-179.78	-359.35
C6	C4	C12	C11	0.6	0.14	-0.46
C4	C6	C7	C9	-0.24	-0.23	0.01
N32	C6	C7	C9	179.85	179.67	-0.18
C4	C6	N32	C55	150.04	143.88	-6.16
C4	C6	N32	C66	-30.2	-35.46	-5.26
C7	C6	N32	C55	-30.05	-36.02	-5.97
C7	C6	N32	C66	149.71	144.64	-5.07
C6	C7	C9	C11	0.55	0.08	-0.47
C7	C9	C11	C12	-0.29	0.17	0.46
C7	C9	C11	C14	179.64	-179.58	-359.22
C9	C11	C12	C4	-0.29	-0.28	0.01
C14	C11	C12	C4	179.79	179.46	-0.33
C9	C11	C14	O1	-177.97	179.92	357.89
C9	C11	C14	N2	1.91	0.27	-1.64
C12	C11	C14	O1	1.95	0.17	-1.78
C12	C11	C14	N2	-178.16	-179.47	-1.31
O1	C15	C30	O16	-179.77	-179.25	0.52
O1	C15	C30	N18	0.5	0.43	-0.07
N3	C15	C30	O16	0.51	0.43	-0.08
N3	C15	C30	N18	-179.21	-179.89	-0.68
C6	N32	C55	C56	133.37	138.28	4.91
C6	N32	C55	C57	-47.53	-41.65	5.88
C66	N32	C55	C56	-46.39	-42.37	4.02
C66	N32	C55	C57	132.7	137.7	5
C6	N32	C66	C67	133.61	137.48	3.87
C6	N32	C66	C68	-47.33	-42.43	4.9
C55	N32	C66	C67	-46.63	-41.86	4.77
C55	N32	C66	C68	132.43	138.22	5.79
N31	C33	C34	C36	178.94	179.81	0.87

N32	C55	C56	C58	178.94	179.81	0.87
C57	C55	C56	C58	-0.17	-0.26	-0.09
N32	C55	C57	C60	-179.85	179.61	359.46
C56	C55	C57	C60	-0.74	-0.32	0.42
C55	C56	C58	C62	0.81	0.6	-0.21
C55	C57	C60	C62	1.03	0.57	-0.46
C56	C58	C62	C60	-0.53	-0.35	0.18
C57	C60	C62	C58	-0.39	-0.24	0.15
N32	C66	C67	C69	178.89	179.8	0.91
C68	C66	C67	C69	-0.18	-0.28	-0.1
N32	C66	C68	C71	-179.81	179.63	359.44
C67	C66	C68	C71	-0.74	-0.28	0.46
C66	C67	C69	C73	0.81	0.6	-0.21
C66	C68	C71	C73	1.03	0.54	-0.49
C67	C69	C73	C71	-0.53	-0.35	0.18
C68	C71	C73	C69	-0.39	-0.23	0.16

Table S4 Calculated bond length of optimized structure of DPAOXDBEN in the ground state and first excited state

Bond		S_0	S_1	variation
O1	C8	1.3593	1.3625	0.0032
O1	C20	1.3588	1.3684	0.0096
N2	C9	1.4045	1.399	-0.0055
N2	C21	1.4217	1.4202	-0.0015
N2	C22	1.4215	1.4199	-0.0016
C3	C9	1.4012	1.4079	0.0067
C3	C10	1.3835	1.3765	-0.007
C5	C15	1.3968	1.4199	0.0231
C5	C17	1.397	1.4195	0.0225
C5	C20	1.4567	1.4154	-0.0413
C6	C9	1.4029	1.4107	0.0078
C6	C13	1.3813	1.3739	-0.0074
C8	C19	1.453	1.4259	-0.0271
C8	N23	1.2951	1.3182	0.0231
C10	C19	1.3956	1.4086	0.013
N12	C20	1.2924	1.3252	0.0328
N12	N23	1.3812	1.3434	-0.0378
C13	C19	1.3976	1.4107	0.0131
C15	C60	1.3835	1.368	-0.0155
C17	C58	1.3835	1.368	-0.0155
C21	C24	1.3963	1.3973	0.001
C21	C26	1.3958	1.3971	0.0013
C22	C28	1.3959	1.3971	0.0012

C22	C34	1.3963	1.3974	0.0011
C24	C36	1.3883	1.3876	-0.0007
C26	C32	1.3883	1.3875	-0.0008
C28	C42	1.3883	1.3874	-0.0009
C30	C32	1.3904	1.391	0.0006
C30	C36	1.3905	1.3909	0.0004
C34	C40	1.3883	1.3875	-0.0008
C38	C40	1.3905	1.391	0.0005
C38	C42	1.3903	1.391	0.0007
C48	C58	1.3968	1.4199	0.0231
C48	C60	1.397	1.4195	0.0225
C48	C63	1.4567	1.4154	-0.0413
C56	C62	1.3976	1.4107	0.0131

Table S5 Calculated angles of optimized structure of DPAOXDBEN in the ground state and first excited state

Angle			S_0	S_1	variation
C8	O1	C20	102.9	103.08	0.18
C9	N2	C21	120.61	120.53	-0.08
C9	N2	C22	120.67	120.54	-0.13
C21	N2	C22	118.72	118.93	0.21
C9	C3	C10	120.62	120.71	0.09
C15	C5	C17	119.83	118.89	-0.94
C15	C5	C20	119.07	119.53	0.46
C17	C5	C20	121.1	121.57	0.47
C9	C6	C13	120.67	120.7	0.03
O1	C8	C19	119.58	120.62	1.04
O1	C8	N23	111.76	111.17	-0.59
C19	C8	N23	128.66	128.21	-0.45
N2	C9	C3	120.75	120.72	-0.03
N2	C9	C6	120.72	120.69	-0.03
C3	C9	C6	118.53	118.59	0.06
C3	C10	C19	120.62	120.72	0.1
C20	N12	N23	106.74	107.4	0.66
C6	C13	C19	120.59	120.73	0.14
C5	C15	C60	120.04	120.53	0.49
C5	C17	C58	120.12	120.57	0.45
C8	C19	C10	121.58	121.59	0.01
C8	C19	C13	119.46	119.86	0.4
C10	C19	C13	118.96	118.55	-0.41
O1	C20	C5	119.64	120.75	1.11
O1	C20	N12	111.9	110.75	-1.15
C5	C20	N12	128.46	128.51	0.05
N2	C21	C24	120.55	120.37	-0.18

N2	C21	C26	120.11	120.15	0.04
C24	C21	C26	119.33	119.48	0.15
N2	C22	C28	120.12	120.17	0.05
N2	C22	C34	120.57	120.38	-0.19
C28	C22	C34	119.3	119.45	0.15
C8	N23	N12	106.7	107.61	0.91
C21	C24	C36	120.14	120.03	-0.11
C21	C26	C32	120.17	120.04	-0.13
C22	C28	C42	120.17	120.05	-0.12
C32	C30	C36	119.42	119.47	0.05
C26	C32	C30	120.46	120.49	0.03
C22	C34	C40	120.16	120.05	-0.11
C24	C36	C30	120.47	120.49	0.02
C40	C38	C42	119.39	119.46	0.07
C34	C40	C38	120.48	120.48	0
C28	C42	C38	120.48	120.5	0.02
C58	C48	C60	119.83	118.89	-0.94
C58	C48	C63	119.07	119.53	0.46
C60	C48	C63	121.1	121.57	0.47
C49	C56	C62	120.59	120.73	0.14
C17	C58	C48	120.04	120.53	0.49
C15	C60	C48	120.12	120.57	0.45

Table S6 Calculated torsion of optimized structure of DPAOXDBEN in the ground state and first excited state

Torsion				S_0	S_1	variation
C20	O1	C8	C19	179.92	179.97	0.05
C20	O1	C8	N23	-0.03	0	0.03
C8	O1	C20	C5	-179.96	-179.98	-0.02
C8	O1	C20	N12	-0.01	-0.02	-0.01
C21	N2	C9	C3	148.28	146.91	-1.37
C21	N2	C9	C6	-31.76	-33.13	-1.37
C22	N2	C9	C3	-31.84	-33.09	-1.25
C22	N2	C9	C6	148.12	146.86	-1.26
C9	N2	C21	C24	-46.72	-44.15	2.57
C9	N2	C21	C26	134.03	136.16	2.13
C22	N2	C21	C24	133.4	135.86	2.46
C22	N2	C21	C26	-45.86	-43.84	2.02
C9	N2	C22	C28	134.44	136.03	1.59
C9	N2	C22	C34	-46.37	-44.32	2.05
C21	N2	C22	C28	-45.68	-43.97	1.71
C21	N2	C22	C34	133.51	135.68	2.17
C10	C3	C9	N2	179.59	179.78	0.19

C10	C3	C9	C6	-0.36	-0.18	0.18
C9	C3	C10	H11	179.76	179.33	-0.43
C9	C3	C10	C19	0.63	0.26	-0.37
C17	C5	C15	C60	0.01	0	-0.01
C20	C5	C15	C60	-179.99	179.98	359.97
C15	C5	C17	C58	-0.01	0	0.01
C20	C5	C17	C58	179.99	-179.98	-359.97
C15	C5	C20	O1	179.94	179.99	0.05
C15	C5	C20	N12	-0.01	0.03	0.04
C17	C5	C20	O1	-0.05	-0.03	0.02
C17	C5	C20	N12	180	-179.99	-359.99
C13	C6	C9	N2	179.82	-179.99	-359.81
C13	C6	C9	C3	-0.23	-0.03	0.2
C9	C6	C13	C19	0.56	0.17	-0.39
O1	C8	C19	C10	1.07	0.46	-0.61
O1	C8	C19	C13	-178.87	-179.5	-0.63
N23	C8	C19	C10	-178.99	-179.58	-0.59
N23	C8	C19	C13	1.07	0.46	-0.61
O1	C8	N23	N12	0.06	0.02	-0.04
C19	C8	N23	N12	-179.89	-179.95	-0.06
C3	C10	C19	C8	179.76	179.91	0.15
C3	C10	C19	C13	-0.3	-0.12	0.18
N23	N12	C20	O1	0.04	0.03	-0.01
N23	N12	C20	C5	179.99	179.99	0
C20	N12	N23	C8	-0.06	-0.03	0.03
C6	C13	C19	C8	179.65	179.87	0.22
C6	C13	C19	C10	-0.3	-0.09	0.21
C5	C15	C60	C48	-0.01	0	0.01
C5	C17	C58	C48	0.01	0	-0.01
N2	C21	C24	C36	-179.98	179.82	359.8
C26	C21	C24	C36	-0.72	-0.48	0.24
N2	C21	C26	C32	179.05	179.51	0.46
C24	C21	C26	C32	-0.21	-0.19	0.02
N2	C22	C28	C42	178.99	179.48	0.49
C34	C22	C28	C42	-0.21	-0.17	0.04
N2	C22	C34	C40	-179.9	179.87	359.77
C28	C22	C34	C40	-0.71	-0.48	0.23
C21	C24	C36	C30	1.04	0.73	-0.31
C21	C26	C32	C30	0.83	0.63	-0.2
C22	C28	C42	C38	0.82	0.62	-0.2
C36	C30	C32	C26	-0.51	-0.39	0.12
C32	C30	C36	C24	-0.43	-0.29	0.14

C22	C34	C40	C38	1.01	0.69	-0.32
C42	C38	C40	C34	-0.4	-0.25	0.15
C40	C38	C42	C28	-0.52	-0.41	0.11

Table S7 Orbital energy of DPAOXD and DPAOXDBEN (eV)

	H-2	H-1	H	L	L+1	L+5	L+6	$\Delta E_{H-1-L+1}$	ΔE_{H-L}	$\Delta E_{H-1-L+5}$	ΔE_{H-L+6}
DPAOXD	-7.98	-6.58	-6.45	-0.72	-0.01	0.87	0.87	6.59	5.73	7.45	7.32
DPAOXDBEN	-7.62	-6.50	-6.41	-0.87	-0.03	0.87	0.88	6.59	5.54	7.37	7.29

Table S8 Calculated atomic charge of different fragment in these compounds invesgated.

	DPAOXD			DPAOXDBEN			BOXD-*p*-OCH_3		
	S_0	S_1	variation	S_0	S_1	variation	S_0	S_1	variation
OXD	-0.20013	-0.36792	-0.16779	-0.22426	-0.30775	-0.08349	-0.18928	-0.33248	-0.1432
c-BEN	/	/	/	0.06306	-0.01922	-0.08228	/	/	/
BEN	0.05736	0.05304	-0.00432	0.03413	0.04762	0.01349	0.21066	0.31028	0.09962
D	0.14169	0.31386	0.17217	0.12714	0.27948	0.15234	-0.02124	0.02236	0.0436