

Recent Breakthroughs in Through-Space Charge Transfer in π -Stacked Molecules as Thermally Activated Delayed Fluorescent Emitters for OLED Applications

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Table S1: Thermal and photophysical data of π -stacked TSCT TADF emitters.

S.No.	Emitter	Thermal data	Photophysical data			Ref
		T_g/T_d (°C) ^a	Radiative decay rate constant (k_r) (10^6 s ⁻¹)	Nonradiative decay rate constant (k_{nr}) (10^6 s ⁻¹)	Reverse intersystem crossing rate constant (k_{RISC}) (10^5 s ⁻¹)	
1	B-oCz	58/303	---	---	---	1
2	B-oTC	105/280	---	---	---	1
3	oB-2Cz	108/334	0.1218	---	5.17	2
4	oB-2tCz	---/380	0.0564	---	17.06	2
5	S-CNDF-S-tCz	--/246	---	---	0.12 ± 0.05	3
6	S-CNDF-D-tCz	--/363	---	---	2.27 ± 0.30	3
7	T-CNDF-T-tCz	--/390	---	---	5.07 ± 0.65	3
8	SF12oTz	--/403	400	---	10.5	4
9	SF23oTz	--/386	120	---	3.8	4
10	SF34oTz	--/370	60	---	1.4	4
11	4Cz-DPS	121/394	---	---	0.89	5
12	2Cz-DPS	111/389	---	---	1.74	5
13	CzTrz	124.6/365.9	---	---	---	6
14	mCzTrz	124.1/309.4	---	---	---	6
15	tCzTrz	127.8/372.8	---	---	---	6
16	CzPhPI	--/280	---	---	---	7
17	CzPhNI	--/310	---	---	---	7
18	v-PXZTRZ	118/453	---	---	23	8
19	v-PTZTRZ	120/408	---	---	20	8
20	l-PXZTRZ	--/447	---	---	6	8
21	l-PTZTRZ	--/451	---	---	8	8
22	DTPA-DTM	117/430	19.9	31.6	6.5	9
23	DTPA-DDTM	170/485	21	13.7	6.7	9
24	tCPT	133.2/387.6	79	0.015	0.15	10
25	Ph-tCPT	140.9/389.1	63	0.011	0.2	10
26	o-PhCz-tCPT	168.3/441.8	51	0.015	0.3	10
27	p-PhCz-tCPT	NA/443.9	46	0.011	0.22	10

28	3-PhCz-tCPT	162.3/435.9	15	0.12	1.7	10
29	PXZ-CTZ	--/422	0.695	0.562	12.8	11
30	DPXZ-CTZ	--/425	0.848	0.246	23.1	11
31	DPXZ-BO	--/408	2.36	0.238	21.0	11
32	Ph ₃ TRZCzTPA	111/324	1.5	---	0.63	12
33	Ph ₂ TRZCzTPA	111/389	3.7	---	1.0	12
34	Ph ₂ TRZCzPhCz	127/340	---	---	---	12
35	Ph ₃ TRZCzPhCz	129/419	---	---	---	12
36	3TCPM	--/367	8.1	1.48	10.5	13
37	2TCPM	148/377	4.3	1.74	9.4	13
38	1TCPM	--/407	8.9	0.87	23.4	13
39	1TCPM-Cz	--/433	9.2	0.69	29.7	13
40	TC	115/403	---	---	---	14
41	PTC	115/377	---	---	---	14
42	PAPTC	103/472	---	---	5.08	14
43	BPAPTC	--/462	---	---	8.43	14
44	2CTC	NA/468	---	---	1.23	15
45	2TBCTC	NA/523	---	---	1.54	15
46	DPXZ-QX	---	1.65	0.579	1.86	16
47	DPXZ-DFQX	---	1.74	0.712	4.33	16
48	DPXZ-2QX	---	0.89	0.133	8.21	16
49	DPXZ-2DFQX	---	2.67	0.264	4.64	16
50	TPA-QX	---	---	---	---	16
51	PXZ-QX	---	---	---	---	16
52	TPXZ-QX	---/420	3.60	5.18	1.75	17
53	TPXZ-2QX	---/472	6.87	14.6	1.53	17
54	2DPXZ-QX	---/472	---	---	3.31	18
55	2DPXZ-DFQX	---/477	---	---	3.51	18
56	BNB-m	---/529	6.12	---	1.60	19
57	BNB-p	---/522	2.86	---	0.988	19
58	NBNN1	NA/378	---	---	2.7	20
59	NBNN2	188/495	---	---	1.2	20
60	TAcBO-H	---	---	---	27	21
61	TAcBO-F	---	---	---	52	21
62	Ac3TRZ3	181/>380	---	---	10	22
63	TAc3TRZ3	175/>380	---	---	21	22
64	BD-Cy	150/--	---	---	86	23
65	YD-TF	161/--	---	---	77	23
66	RD-2TF	153/--	---	---	19	23
67	TRZ-o-SDMAC	--/>435	---	---	---	24
68	TRZ-m-SDMAC	--/>435	---	---	---	24
69	TRZ-p-SDMAC	--/>435	---	---	---	24
70	XPT	101/318	---	---	---	25
71	XCT	109/312	---	---	---	25
72	XtBuCT	132/313	---	---	---	25
73	DMAC-TPA-TRZ	141/372	---	---	---	26
74	DMAC-Ph-TRZ	---/315	---	---	---	26
75	PXZ-TPA-TRZ	122/361	---	---	0.764	26
76	PXZ-Ph-TRZ	---/303	---	---	1.48	26
77	TPA-ace	---	---	---	---	27
78	TPA-ace-Br	---	---	---	---	27
79	2TPA-ace	---	---	---	---	27
80	TPA-ace-CN	---	---	---	---	27
81	TPA-ace-TRZ	---	---	---	---	27
82	BF-oTCz	227/---	---	---	0.6	28
83	BF-oPCz	290/---	---	---	0.5	28
84	BF-oTMCz	335/---	---	---	22.7	28

^a T_g: Glass transition temperature and T_d: decomposition temperature.

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