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Electronic Supplementary Information

New insights into Two-Photon Absorption Properties of Functionalized Aza-BODIPY Dyes at Telecommunication Wavelengths: a Theoretical Study

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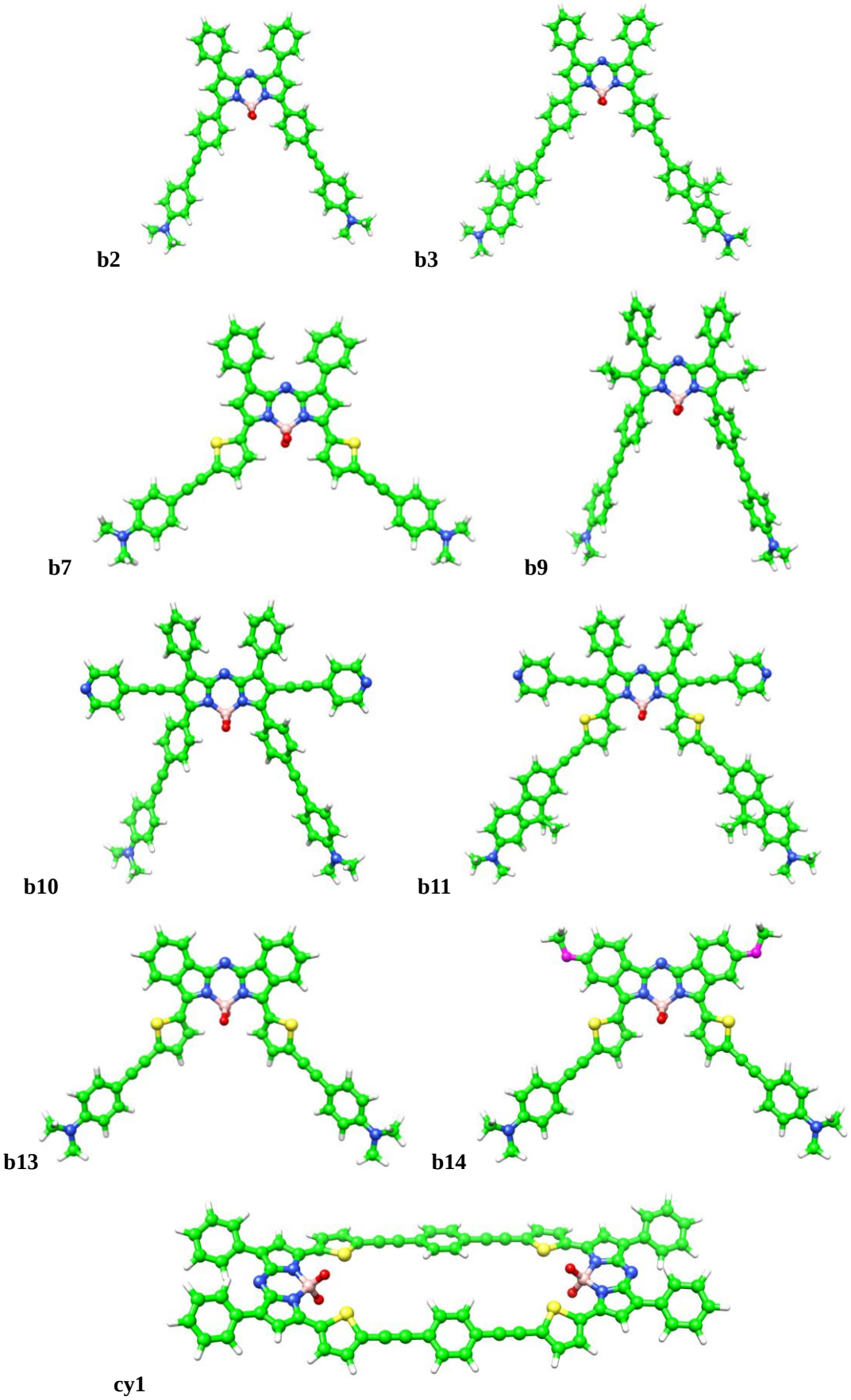
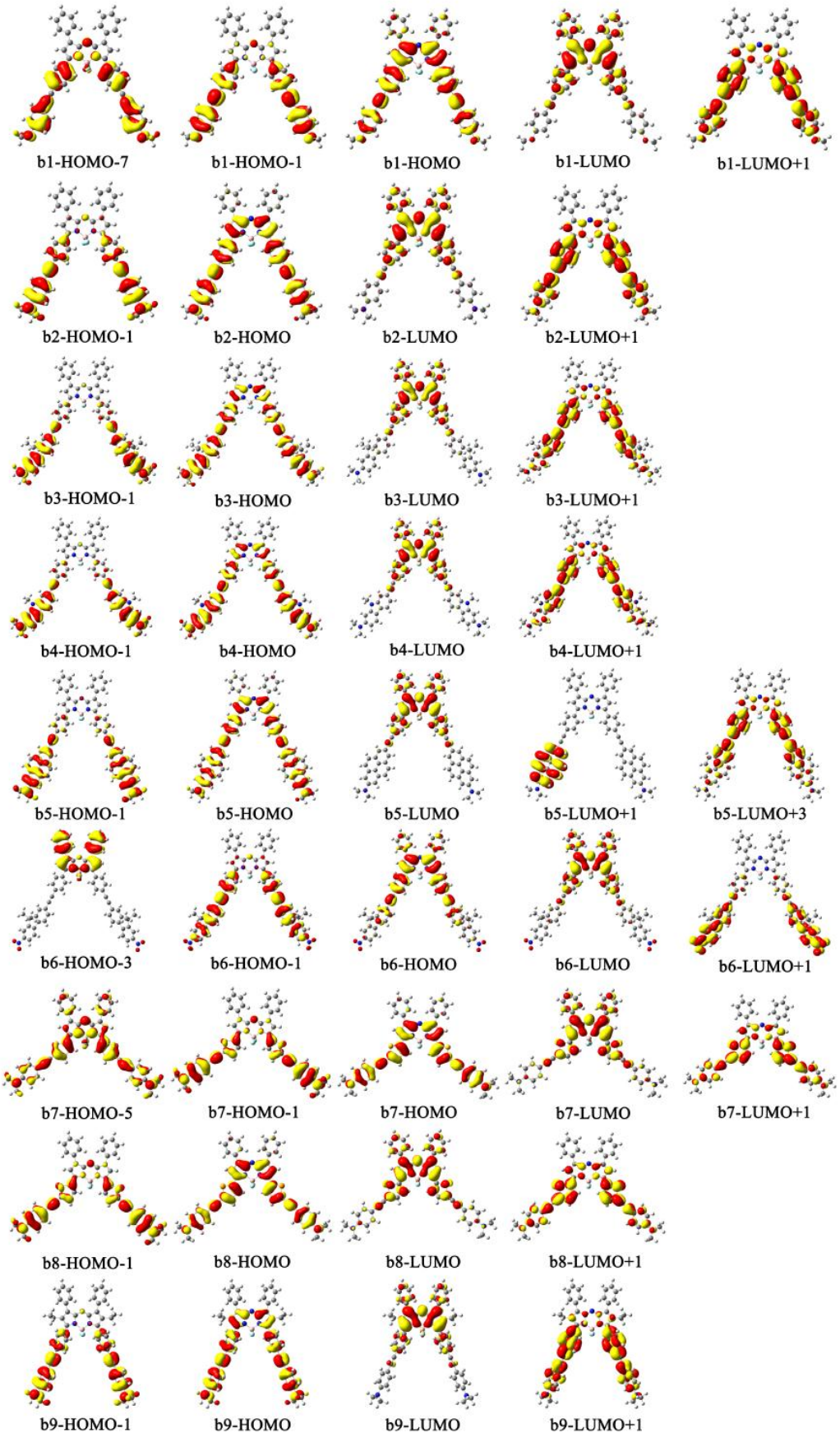


Fig. S1 The optimized ground-state geometries of all chromophores



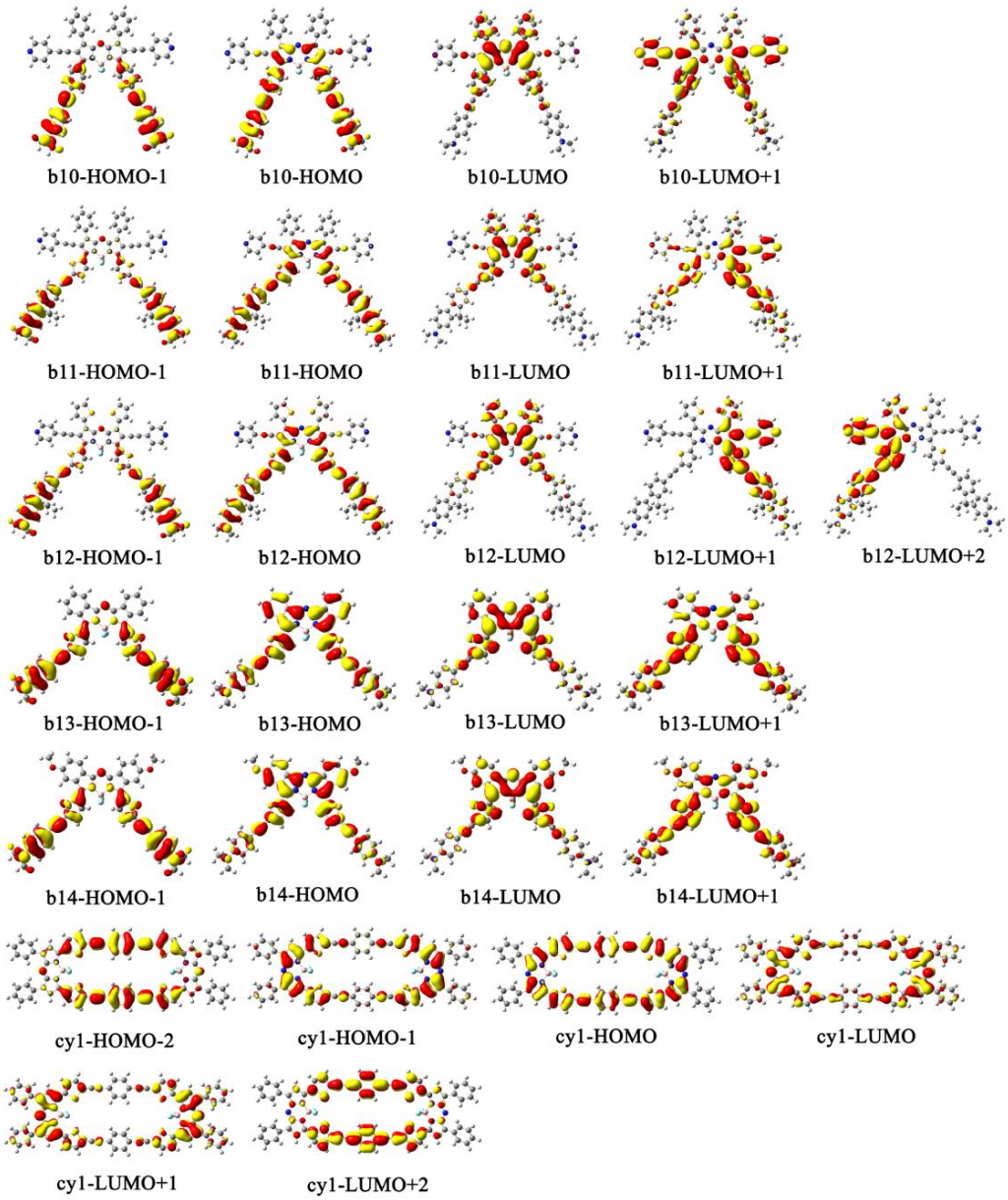


Fig. S2 Contour surfaces of the frontier molecular orbitals relevant to the maximal one- and two-photon absorptions.

Table S1 One- and two-photon absorption properties (ZINDO), λ^{T}_{max}/nm, δ_{max}/GM.

Mol.	λ^{O}_{max}	f	Transition characteristics	λ^{T}_{max}	δ_{max}	Transition channel and nature
b1	737.1	0.65	$S_0 \rightarrow S_1$ (H)→(L)80%	1011.3	728.0	$S_0 \rightarrow S_1 \rightarrow S_3$ (H-3)→(L)36% (H-1)→(L)12%
	408.9	0.89	$S_0 \rightarrow S_9$ (H)→(L+1)18%			(H-4, H)→(L, L)12%
			(H)→(L+3)11%	856.3	3688.5	$S_0 \rightarrow S_1 \rightarrow S_8$ (H-1)→(L)38% (H-3)→(L)11%
b2	748.1	0.66	$S_0 \rightarrow S_1$ (H)→(L)81%	1006.4	1252.1	$S_0 \rightarrow S_1 \rightarrow S_3$ (H-3)→(L)32% (H-1)→(L)19%
	415.5	0.82	$S_0 \rightarrow S_{10}$ (H)→(L+1)19%			(H-4, H)→(L, L)10%
				867.0	3641.9	$S_0 \rightarrow S_1 \rightarrow S_8$ (H-1)→(L)35% (H-5)→(L)15%
b3	752.5	0.72	$S_0 \rightarrow S_1$ (H)→(L)82%	1097.2	630.4	$S_0 \rightarrow S_1 \rightarrow S_2$ (H, H)→(L, L)46%
	419.0	0.94	$S_0 \rightarrow S_6$ (H-5)→(L)24%	968.6	2697.1	$S_0 \rightarrow S_1 \rightarrow S_4$ (H-1)→(L)35% (H-3)→(L)20%
			(H)→(L+1)13%			
b4	761.5	0.71	$S_0 \rightarrow S_1$ (H)→(L)82%	1109.0	561.5	$S_0 \rightarrow S_1 \rightarrow S_2$ (H, H)→(L, L)46%
	460.8	1.03	$S_0 \rightarrow S_4$ (H-1)→(L)38%	925.3	3720.5	$S_0 \rightarrow S_1 \rightarrow S_4$ (H-1)→(L)38%
b5	613.0	0.79	$S_0 \rightarrow S_1$ (H)→(L)80%	991.9	358.5	$S_0 \rightarrow S_1 \rightarrow S_2$ (H, H)→(L, L)48%
	408.2	1.34	$S_0 \rightarrow S_7$ (H-3)→(L)24%	809.3	1808.9	$S_0 \rightarrow S_1 \rightarrow S_7$ (H-3)→(L)24% (H-5)→(L)23%
			(H-5)→(L)23%			(H-7)→(L)21%
			(H-7)→(L)21%			
b6	709.1	0.66	$S_0 \rightarrow S_1$ (H)→(L)88%	1103.1	540.7	$S_0 \rightarrow S_1 \rightarrow S_2$ (H, H)→(L, L)49% (H)→(L+5)12%
	423.7	1.21	$S_0 \rightarrow S_9$ (H-1)→(L)12%	996.7	607.1	$S_0 \rightarrow S_1 \rightarrow S_6$ (H-3)→(L)45% (H-1)→(L)16%
			(H-2)→(L+1)12%			(H-4, H)→(L, L)11%
			(H-1)→(L+2)12%	856.3	2564.2	$S_0 \rightarrow S_1 \rightarrow S_8$ (H-1,H)→(L,L+3)11%
b7	802.4	0.85	$S_0 \rightarrow S_1$ (H)→(L)79%	1026.4	5312.3	$S_0 \rightarrow S_1 \rightarrow S_4$ (H-1)→(L)26% (H, H)→(L, L)19%
	472.3	0.80	$S_0 \rightarrow S_5$ (H)→(L+1)16%			
			(H-3)→(L)14%			
b8	799.9	0.85	$S_0 \rightarrow S_1$ (H)→(L)81%	1026.4	5200.3	$S_0 \rightarrow S_1 \rightarrow S_4$ (H-1)→(L)27% (H, H)→(L, L)18%
	469.6	0.86	$S_0 \rightarrow S_5$ (H)→(L+1)16%			
			(H-3)→(L)12%			
b9	691.1	0.56	$S_0 \rightarrow S_1$ (H)→(L)79%	977.8	539.1	$S_0 \rightarrow S_1 \rightarrow S_3$ (H-3)→(L)32% (H-4, H)→(L, L)12%
	404.1	0.57	$S_0 \rightarrow S_{10}$ (H)→(L+1)13%	863.4	1307.3	$S_0 \rightarrow S_1 \rightarrow S_7$ (H-1)→(L)44% (H-5)→(L)13%
			(H-1)→(L+2)14%			
b10	812.0	0.78	$S_0 \rightarrow S_1$ (H)→(L)79%	1080.0	1582.7	$S_0 \rightarrow S_1 \rightarrow S_4$ (H, H)→(L, L)27%
	470.5	0.60	$S_0 \rightarrow S_5$ (H-1)→(L)55%	942.1	3602.8	$S_0 \rightarrow S_1 \rightarrow S_5$ (H-1)→(L)55%
b11	878.4	0.87	$S_0 \rightarrow S_1$ (H)→(L)84%	1115.0	4637.8	$S_0 \rightarrow S_1 \rightarrow S_4$ (H-3)→(L)31% (H-1)→(L)14%
	559.5	0.69	$S_0 \rightarrow S_4$ (H-3)→(L)31%	973.2	7235.3	$S_0 \rightarrow S_1 \rightarrow S_7$ (H)→(L+1)22% (H, H)→(L, L)18%
			(H-1)→(L)14%			
b12	941.4	0.81	$S_0 \rightarrow S_1$ (H)→(L)79%	1280.8	2099	$S_0 \rightarrow S_1 \rightarrow S_4$ (H-3)→(L)16% (H, H)→(L, L)20%
	509.3	1.28	$S_0 \rightarrow S_6$ (H)→(L+1)30%			
			(H-1)→(L)21%			
b13	926.4	0.58	$S_0 \rightarrow S_1$ (H)→(L)67%	1610.2	127.2	$S_0 \rightarrow S_1 \rightarrow S_2$ (H, H)→(L, L)36% (H)→(L+1)25%
			(H, H)→(L, L+2)16%	1178.6	1827.4	$S_0 \rightarrow S_1 \rightarrow S_4$ (H)→(L+3)19% (H-1)→(L)12%
	476.6	0.94	$S_0 \rightarrow S_5$ (H-1)→(L)27%			(H, H)→(L, L+2)11%
			(H)→(L+1)26%			
b14	948.2	0.58	$S_0 \rightarrow S_1$ (H)→(L)68%	1662.0	187.4	$S_0 \rightarrow S_1 \rightarrow S_2$ (H, H)→(L, L)40% (H)→(L+1)23%
			(H, H)→(L, L+1)16%	1206.1	1323.3	$S_0 \rightarrow S_1 \rightarrow S_4$ (H)→(L+3)17% (H-1)→(L)13%

	473.8	1.00	$S_0 \rightarrow S_6$ (H)→(L+1)30% (H-1)→(L)25%			(H, H)→(L, L+2)13%	(H-2, H)→(L, L)12%
cy1	663.3	1.22	$S_0 \rightarrow S_3$ (H-1)→(L)41% (H)→(L+1)47%	1031.5 897.1	740.5 4420.3	$S_0 \rightarrow S_3 \rightarrow S_7$ (H-3)→(L)18% $S_0 \rightarrow S_3 \rightarrow S_{11}$ (H-2)→(L+1)30%	(H)→(L+3)10%
	461.6	2.03	$S_0 \rightarrow S_{10}$ (H-2)→(L)41%			(H-1, H)→(L, L+1)12%	
	423.4	2.29	$S_0 \rightarrow S_{13}$ (H)→(L+2)30%				