Supporting Information

Effect of Regio-specific Arylamine Substitution on Novel π-extended Zinc Salophen Complexes: Density Functional and Time-dependent Density Functional Study Prompted for DSSC Applications

Jian-Ming Liao, Yu-Kai Chin, Yu-Ting Wu and Hsien-Hsin Chou*

Department of Applied Chemistry, Providence University, Taichung 43301, Taiwan

AUTHOR INFORMATION

Corresponding Author

*E-mail: hhchou@pu.edu.tw

Table S2. Gas-phase TDDFT results for ZSC dyes calculated at B3LYP/6-311G(d,p) level of theory.

YD-H					YD-AN				
	eV	nm	f			eV	nm	f	
S1	2.5876	479.15	0.5061	H→L 96%	S1	2.2149	559.78	0.1358	H→L 97%
S2	2.7766	446.54	0.0099	H1→L 85%	S2	2.52	492	0.1154	H1→L 9%
				H→L1 11%					H→L1 88%
S3	2.9948	414	0.147	H1→L 9%	S3	2.6642	465.37	0.448	H1→L 87%
				H1→L1 6%					H→L1 9%
				H→L1 83%	S4	2.8686	432.21	0.0011	H→L2 98%
S4	3.1316	395.92	0.1914	H1→L 3%	S5	2.981	415.91	0.0659	H2→L 23%
				H1→L1 88%					H1→L1 74%
				H→L1 3%	S6	3.0753	403.16	0.1654	H2→L 72%
S5	3.296	376.16	0.8236	H2→L 13%					H1→L1 24%
				H→L2 85%	S7	3.3049	375.15	0.8845	H3→L 10%
S6	3.4153	363.03	0.0204	H3→L 77%					H2→L1 6%
				H2→L 8%					H1→L2 81%
				H1→L2 5%	S8	3.3627	368.7	0.3043	H6→L 3%
				H→L2 3%					H2→L1 87%
S7	3.4301	361.46	0.1697	H3→L 14%					H1→L2 5%
				H3→L1 2%	S9	3.4128	363.29	0.0085	H4→L 90%
				H2→L 50%					H4→L1 2%
				H1→L2 23%	S10	3.4632	358.01	0.0518	H3→L 82%
				H→L2 7%					H1→L2 10%
S8	3.4903	355.22	0.1185	H2→L 23%	S11	3.6764	337.24	0.0802	H4→L1 15%
				H1→L2 70%					H3→L1 7%
				H→L2 2%					H2→L2 72%
S9	3.6653	338.26	0.0422	H8→L 3%	S12	3.6849	336.46	0.0415	H10→L 4%
				H4→L 6%					H6→L 3%
				H3→L1 27%					H4→L1 39%
				H2→L1 57%					H3→L 2%
S10	3.7145	333.78	0.0596	H8→L 3%					H3→L1 22%

State	E (eV)	λ (nm)	f	Transition	%	State	E (eV)	λ (nm)	f	Transition	%
				H7→L	5%					H2→L2	24%
				H4→L	3%	S13	3.7244	332.9	0.1062	H9→L	3%
				H3→L1	54%					H6→L	3%
				H2→L1	29%					H4→L1	27%
S11	4.0275	307.84	0.3545	H4→L	49%					H3→L1	59%
				H2→L1	4%	S14	4.023	308.19	0.4139	H6→L	54%
				H2→L2	41%					H5→L	14%
S12	4.0697	304.65	0.2607	H4→L	33%					H3→L1	4%
				H2→L1	6%					H3→L2	16%
				H2→L2	54%					H2→L1	3%
S13	4.1476	298.93	0.102	H8→L	3%					H→L4	2%
				H5→L	88%	S15	4.0682	304.77	0.1552	H6→L	6%
S14	4.2511	291.65	0.0215	H8→L	27%					H5→L	4%
				H7→L	47%					H3→L1	2%
				H5→L	5%					H3→L2	76%
				H3→L	3%					H→L4	4%
				H3→L1	10%	S16	4.0904	303.11	0.0137	H6→L	21%
				H3→L2	2%					H5→L	63%
S15	4.H153	289.39	0.0605	H5→L1	3%					H5→L1	10%
				H4→L1	89%					H→L7	2%
S16	4.3619	H15.25	0	H6→L	7%	S17	4.1252	300.55	0.0631	H7→L	4%
				H6→L2	19%					H6→L	2%
				H1→L3	10%					H5→L	5%
				H→L3	59%					H→L4	76%
S17	4.4342	279.61	0.0001	H7→L	4%					H→L7	6%
				H3→L2	89%	S18	4.1589	298.12	0.1338	H10→L	6%
S18	4.4647	277.7	0.0253	H10→L	8%					H7→L	79%
				H4→L1	3%					H4→L1	2%
				H→L4	75%					H→L4	3%
S19	4.5138	274.68	0.0452	H9→L	11%	S19	4.2109	294.44	0.0329	H→L4	8%

State	eV	nm	f	Transition	%	State	eV	nm	f	Transition	%
				H9→L2	4%					H→L6	5%
				H8→L	46%					H→L7	73%
				H7→L	28%	S20	4.2435	292.18	0.0325	H10→L	40%
				H→L6	2%					H9→L	29%
S20	4.5177	274.44	0.0108	139→L	2%					H7→L	9%
				H9→L	53%					H4→L	4%
				H9→L1	4%					H4→L1	9%
				H9→L2	23%					H4→L2	3%
				H8→L	10%						
				H7→L	5%						

YD-DPA						YD-TPA					
	eV	nm	*f*				eV	nm	*f*		
S1	2.1573	574.71	0.1709	H→L	96%	S1	2.265	547.4	0.1465	H→L	95%
				H→L1	2%	S2	2.5506	486.09	0.1368	H1→L	14%
S2	2.4927	497.39	0.0399	H1→L	5%					H→L1	81%
				H→L	2%	S3	2.6304	471.36	0.4109	H1→L	81%
				H→L1	90%					H→L1	15%
S3	2.5975	477.32	0.4546	H1→L	92%	S4	2.8655	432.68	0.0402	H2→L	79%
				H→L1	5%					H1→L1	14%
S4	2.8981	427.81	0.0082	H1→L1	5%	S5	2.9472	420.69	0.0024	H1→L1	4%
				H→L2	94%					H→L2	95%
S5	2.9249	423.89	0.1662	H2→L	7%	S6	2.9849	415.38	0.1367	H2→L	15%
				H1→L1	85%					H1→L1	77%
				H→L2	5%					H→L2	3%
S6	3.1074	399	0.3399	H2→L	87%	S7	3.1801	389.88	0.1411	H2→L1	92%
				H1→L1	7%	S8	3.3053	375.11	1.2482	H3→L	26%
S7	3.3027	375.41	0.7067	H3→L	4%					H1→L2	69%
				H2→L1	5%	S9	3.4131	363.26	0.0195	H5→L	63%
				H1→L2	88%					H3→L	16%
S8	3.3846	366.32	0.1968	H5→L	4%					H1→L2	11%

State	eV	nm	f	Transition	%
				H3→L	5%
				H2→L1	83%
				H1→L2	3%
S9	3.4249	362.01	0.0028	H12→L1	3%
				H4→L	93%
S10	3.5064	353.59	0.0919	H3→L	82%
				H3→L1	2%
				H2→L1	2%
				H1→L2	5%
S11	3.7227	333.05	0.2136	H4→L1	5%
				H3→L1	2%
				H2→L2	86%
S12	3.7365	331.82	0.0018	H12→L	12%
				H11→L	2%
				H4→L1	70%
				H4→L2	2%
				H2→L2	4%
				H→L3	2%
S13	3.757	330.01	0.0177	H3→L1	5%
				H→L3	78%
				H→L4	2%
				H→L6	5%
S14	3.7968	326.55	0.0048	H5→L	3%
				H3→L	2%
				H3→L1	81%
				H→L3	6%
S15	3.9136	316.8	0.1841	H5→L	2%
				H→L3	3%
				H→L4	91%
S16	4.0041	309.64	0.464	H5→L	76%
				H3→L1	2%

State	eV	nm	f	Transition	%
S10	3.4315	361.31	0.0318	H5→L	27%
				H5→L1	3%
				H3→L	49%
				H1→L2	16%
S11	3.555	348.76	0.1314	H3→L	2%
				H2→L2	94%
S12	3.6357	341.02	0.3979	H8→L	2%
				H3→L1	69%
				H→L3	22%
S13	3.6774	337.15	0.0207	H→L3	3%
				H→L4	89%
S14	3.6886	336.12	0.1314	H14→L	7%
				H5→L1	60%
				H→L3	17%
				H→L4	4%
S15	3.7149	333.75	0.1611	H14→L	3%
				H8→L	3%
				H5→L1	18%
				H3→L	2%
				H3→L1	15%
				H→L3	51%
S16	3.9251	315.88	0.1885	H→L5	95%
S17	4.0216	308.29	0.305	H8→L	21%
				H6→L	17%
				H3→L1	3%
				H3→L2	52%
S18	4.0623	305.21	0.2688	H8→L	23%
				H6→L	17%
				H3→L1	6%
				H3→L2	43%
S19	4.1402	299.47	0.0869	H9→L	64%

State	eV	nm	f	Transition	%	State	eV	nm	f	Transition	%
				H2→L1	5%					H7→L	21%
				H→L4	2%					H→L7	2%
				H→L6	3%	S20	4.1426	299.29	0.0321	H9→L	22%
S17	4.1105	301.63	0.0318	H6→L	77%					H7→L	58%
				H6→L1	5%					H7→L1	6%
				H→L8	10%					H6→L	6%
S18	4.1451	299.11	0.1666	H8→L	4%						
				H7→L	65%						
				H7→L1	2%						
				H6→L	4%						
				H5→L	3%						
				H→L6	11%						
S19	4.1642	297.74	0.0216	H7→L	16%						
				H5→L	2%						
				H→L3	5%						
				H→L6	61%						
S20	4.1915	295.8	0.0612	H8→L	24%						
				H6→L	8%						
				H5→L1	3%						
				H3→L2	2%						
				H→L8	49%						
				H→L9	3%						

CL-H						CL-AN					
	eV	nm	f				eV	nm	f		
S1	2.5681	482.78	0.5795	H→L	98%	S1	2.2573	549.27	0.3987	H→L	98%
S2	2.7411	452.31	0.008	H1→L	59%	S2	2.4151	513.38	0.2774	H1→L	8%
				H→L1	39%					H→L1	88%
S3	2.9319	422.88	0.0035	H1→L1	97%	S3	2.6296	471.5	0.6169	H1→L	89%
S4	2.945	421	0.4958	H3→L	3%					H→L1	9%
				H1→L	39%	S4	2.6934	460.33	0.2275	H2→L	89%

State	E (eV)	λ (nm)	f	Transition	%
				H→L1	55%
S5	3.141	394.73	0.5925	H2→L	96%
S6	3.2227	384.72	0.0044	H4→L	82%
				H4→L2	2%
				H3→L	7%
				H2→L1	3%
S7	3.3015	375.54	0.3824	H4→L	10%
				H3→L	71%
				H2→L1	15%
S8	3.3811	366.69	0.3117	H8→L	3%
				H4→L1	41%
				H3→L	2%
				H3→L1	37%
				H2→L1	10%
S9	3.3848	366.29	0.8942	H4→L1	6%
				H3→L	14%
				H3→L1	6%
				H2→L1	68%
S10	3.4381	360.62	0.1443	H8→L	3%
				H4→L1	35%
				H3→L1	52%
				H2→L	2%
S11	3.6227	342.24	0.0085	H5→L	3%
				H1→L3	11%
				H→L2	80%
S12	3.6461	340.04	0.0786	H6→L	3%
				H1→L2	2%
				H→L3	89%
S13	3.791	327.04	0.1245	H1→L2	86%
				H1→L3	2%
				H→L2	2%

State	E (eV)	λ (nm)	f	Transition	%
S5	2.7781	446.29	0.0199	H1→L1	8%
				H3→L1	2%
				H2→L	9%
S6	2.8323	437.75	0.002	H1→L1	87%
				H3→L	78%
				H2→L1	18%
S7	2.9821	415.76	0.2871	H3→L	18%
				H2→L1	77%
S8	2.9911	414.51	0.0066	H3→L1	94%
				H1→L1	3%
S9	3.1697	391.15	0.6034	H4→L	94%
S10	3.213	385.88	0.0375	H11→L1	2%
				H6→L	74%
				H6→L2	3%
				H5→L	4%
				H→L2	11%
				H→L3	3%
S11	3.2205	384.98	0.2384	H5→L	2%
				H→L2	10%
				H→L3	82%
S12	3.2339	383.39	0.041	H6→L	12%
				H→L2	74%
				H→L3	7%
S13	3.3251	372.87	0.4988	H6→L	4%
				H5→L	81%
				H4→L1	9%
S14	3.3942	365.28	0.2607	H11→L	6%
				H6→L1	58%
				H6→L3	3%
				H5→L1	13%
				H4→L1	14%

State	Energy (eV)	λ (nm)	f	Transition	%
				H→L3	2%
S14	3.8045	325.89	0.029	H5→L	2%
				H1→L2	3%
				H1→L3	80%
				H→L2	9%
S15	3.92	316.29	0.0063	H8→L	3%
				H5→L	76%
				H4→L1	5%
				H2→L2	3%
				H→L2	3%
S16	4.0094	309.23	0.0002	H8→L1	3%
				H6→L	12%
				H5→L1	71%
				H3→L2	4%
S17	4.0579	305.54	0.0054	H10→L1	2%
				H9→L	2%
				H8→L	51%
				H7→L	22%
				H5→L	5%
				H4→L1	7%
				H2→L2	4%
S18	4.0954	302.74	0.1285	H6→L	36%
				H5→L1	3%
				H3→L2	12%
				H2→L3	41%
S19	4.1596	298.06	0.0591	H11→L	2%
				H10→L1	2%
				H8→L	2%
				H5→L	7%
				H3→L3	8%

State	Energy (eV)	λ (nm)	f	Transition	%
S15	3.4113	363.45	0.7529	H6→L1	11%
				H5→L	6%
				H5→L1	3%
				H4→L1	70%
				H→L3	2%
S16	3.4768	356.6	0.206	H6→L1	13%
				H5→L1	78%
				H4→L	2%
S17	3.5666	347.63	0.0883	H3→L2	6%
				H2→L3	3%
				H1→L2	79%
				H1→L3	7%
S18	3.5773	346.59	0.0182	H3→L3	5%
				H2→L2	9%
				H1→L2	7%
				H1→L3	74%
S19	3.689	336.09	0.0002	H3→L3	9%
				H2→L2	70%
				H1→L3	16%
S20	3.7254	332.81	0.0567	H3→L2	4%
				H2→L3	83%
				H1→L2	5%

	eV	nm	f		
				H2→L2	65%
				H2→L3	3%
S20	4.1691	297.39	0.0006	H13→L1	2%
				H12→L	4%
				H11→L1	13%
				H10→L	38%
				H8→L1	19%
				H7→L1	8%

CL-DPA						CL-TPA					
	eV	nm	f				eV	nm	f		
S1	2.3154	535.46	0.3186	H→L	94%	S1	2.2654	547.29	0.32	H→L	97%
				H→L1	3%	S2	2.4089	514.69	0.1462	H1→L	20%
S2	2.4696	502.04	0.3692	H2→L	4%					H→L1	77%
				H1→L	17%	S3	2.4879	498.35	0.5015	H1→L	79%
				H→L	3%					H→L1	20%
				H→L1	73%	S4	2.6069	475.6	0.3512	H2→L	77%
S3	2.5212	491.76	0.2188	H1→L	81%					H1→L1	19%
				H→L1	15%	S5	2.6443	468.88	0.0015	H2→L	19%
S4	2.6237	472.55	0.0246	H1→L1	94%					H1→L1	79%
				H1→L2	2%	S6	2.759	449.38	0.0133	H3→L	67%
S5	2.7449	451.69	0.4635	H3→L	5%					H2→L1	29%
				H2→L	84%	S7	2.9194	424.7	0.7122	H3→L	29%
				H→L1	5%					H2→L1	66%
S6	2.8348	437.36	0.0102	H3→L	76%	S8	2.9242	423.99	0.0033	H3→L1	96%
				H2→L	3%	S9	3.1295	396.18	0.5487	H4→L	96%
				H2→L1	19%	S10	3.2065	386.67	0.0176	H7→L	13%
S7	2.902	427.24	0.1362	H3→L	13%					H6→L	67%
				H3→L1	13%					H5→L	5%
				H2→L1	70%					H→L2	5%
S8	3.0229	410.14	0.1164	H3→L	4%	S11	3.2226	384.74	0.1529	H6→L	6%

State	Energy (eV)	λ (nm)	f	Transition	Contribution
				H3→L1	81%
				H2→L	2%
				H2→L1	7%
S9	3.1453	394.19	0.5938	H4→L	94%
S10	3.2228	384.71	0.0872	H6→L	69%
				H5→L	17%
				H4→L1	3%
S11	3.2853	377.4	0.6224	H6→L	15%
				H5→L	53%
				H→L2	18%
				H→L3	9%
S12	3.3124	374.3	0.007	H6→L	4%
				H5→L	16%
				H4→L1	16%
				H→L2	55%
				H→L3	4%
S13	3.3472	370.41	0.3995	H6→L1	6%
				H5→L1	27%
				H4→L1	15%
				H→L2	11%
				H→L3	36%
S14	3.3713	367.76	0.4603	H6→L1	7%
				H5→L	5%
				H5→L1	20%
				H4→L1	54%
				H→L2	7%
S15	3.3844	366.34	0.0873	H15→L	2%
				H6→L1	45%
				H5→L	3%
				H5→L1	2%
				H4→L1	7%

State	Energy (eV)	λ (nm)	f	Transition	Contribution
				H→L2	84%
				H→L4	4%
S12	3.2337	383.41	0.6946	H5→L	23%
				H4→L1	3%
				H→L2	3%
				H→L3	65%
S13	3.2713	379	0.3784	H6→L	3%
				H5→L	60%
				H4→L1	8%
				H1→L2	3%
				H→L3	20%
S14	3.3471	370.43	0.6372	H4→L1	79%
				H1→L2	6%
				H→L3	7%
S15	3.3758	367.27	0.1488	H15→L	2%
				H14→L	2%
				H7→L1	8%
				H6→L1	47%
				H5→L1	32%
S16	3.4246	362.04	0.1334	H7→L1	4%
				H6→L1	23%
				H5→L1	62%
				H4→L	2%
S17	3.4463	359.76	0.005	H5→L	4%
				H4→L1	3%
				H1→L2	83%
S18	3.4614	358.19	0.025	H1→L3	91%
				H→L4	2%
S19	3.5809	346.23	0.0582	H7→L	4%
				H3→L3	5%
				H2→L2	37%

				H→L3	31%						H→L4	45%
S16	3.4503	359.35	0.1537	H6→L1	24%	S20	3.6317	341.4	0.0759	H7→L	6%
				H5→L1	46%					H3→L3	3%
				H→L3	14%					H2→L2	36%
S17	3.5128	352.95	0.0029	H1→L1	3%					H1→L3	3%
				H1→L2	72%					H→L2	3%
				H1→L3	20%					H→L4	37%
S18	3.5672	347.57	0.0048	H1→L2	19%						
				H1→L3	75%						
				H1→L5	2%						
S19	3.6746	337.41	0.0725	H4→L2	2%						
				H2→L2	90%						
S20	3.7809	327.92	0.0724	H7→L	10%						
				H3→L3	16%						
				H2→L3	66%						

AJ1-H (AJ2-H)						AJ1-AN					
	eV	nm	f				eV	nm	f		
S1	2.5522	485.79	0.37	H→L	97%	S1	2.3029	538.38	0.6368	H→L	96%
S2	2.6224	472.79	0.0002	H1→L	64%	S2	2.439	508.35	0.0806	H3→L	2%
				H→L1	34%					H1→L	85%
S3	2.8372	436.99	1.0665	H1→L	34%					H→L1	10%
				H→L1	63%	S3	2.5267	490.7	0.6787	H3→L	19%
S4	2.8816	430.26	0.0199	H1→L1	98%					H2→L1	4%
S5	3.1113	398.49	0.1675	H2→L	42%					H1→L	14%
				H→L2	55%					H→L1	61%
S6	3.1504	393.55	0.1818	H2→L	55%	S4	2.6034	476.24	0.0702	H2→L	94%
				H→L2	43%	S5	2.6764	463.26	0.9205	H3→L	70%
S7	3.2551	380.89	0.0606	H7→L1	2%					H2→L1	3%
				H4→L	58%					H→L1	26%
				H4→L2	9%	S6	2.6813	462.41	0.1966	H1→L1	96%

State	E (eV)	λ (nm)	f	Transition	%	State	E (eV)	λ (nm)	f	Transition	%
				H3→L	26%	S7	2.8465	435.57	0.0158	H3→L1	95%
S8	3.2991	375.81	0.009	H4→L	7%	S8	2.8586	433.72	0.2739	H3→L	6%
				H3→L	10%					H2→L1	88%
				H2→L1	76%	S9	2.8734	431.49	0.0591	H2→L2	5%
				H1→L2	3%					H→L2	92%
S9	3.3499	370.12	0.0264	H1→L2	88%	S10	3.0661	404.37	0.1657	H1→L2	95%
				H→L3	7%					H→L3	2%
S10	3.4401	360.41	0.0053	H7→L	6%	S11	3.1392	394.95	0.322	H4→L	79%
				H7→L2	3%					H2→L2	16%
				H4→L1	64%	S12	3.1971	387.81	0.1779	H5→L	13%
				H4→L3	4%					H3→L2	16%
				H3→L1	19%					H2→L2	3%
S11	3.4876	355.5	0.6642	H4→L	11%					H→L3	60%
				H3→L	29%	S13	3.2094	386.32	0.0049	H4→L	16%
				H2→L1	11%					H2→L2	73%
				H1→L2	2%					H→L2	4%
				H→L3	44%					H→L3	3%
S12	3.5482	349.43	0.6136	H6→L	2%	S14	3.226	384.32	0.0335	H6→L	24%
				H4→L	9%					H6→L2	4%
				H3→L	27%					H5→L	47%
				H2→L1	7%					H5→L2	6%
				H1→L2	4%					H3→L2	4%
				H→L3	43%					H→L3	9%
S13	3.6684	337.98	0.0225	H1→L3	97%	S15	3.2885	377.03	0.1849	H4→L1	8%
S14	3.7361	331.85	0.0988	H5→L	17%					H3→L2	72%
				H4→L1	17%					H→L3	17%
				H3→L1	42%	S16	3.3292	372.41	0.0088	H6→L	16%
				H2→L2	21%					H5→L	7%
S15	3.774	328.52	0.0259	H4→L1	2%					H4→L1	66%
				H3→L1	19%					H3→L2	3%
				H2→L2	73%	S17	3.342	370.99	0.0196	H5→L1	2%

	eV	nm	f				eV	nm	f		
S16	3.8063	325.74	0.0006	H5→L	78%					H1→L3	93%
				H3→L1	16%	S18	3.4077	363.83	0.0000	H11→L	4%
S17	4.0201	308.41	0.0119	H10→L	2%					H11→L2	2%
				H7→L1	15%					H6→L1	28%
				H4→L	12%					H6→L3	2%
				H4→L2	41%					H5→L1	50%
				H3→L2	22%					H5→L3	3%
S18	4.0415	306.78	0.0066	H7→L	61%					H1→L3	5%
				H7→L2	6%	S19	3.5179	352.44	0.0334	H6→L	2%
				H6→L	9%					H4→L1	3%
				H4→L1	7%					H2→L3	88%
				H2→L3	11%					H→L3	3%
S19	4.0491	306.21	0.0054	H7→L	15%	S20	3.5587	348.4	0.7634	H6→L	42%
				H6→L	12%					H5→L	20%
				H5→L1	26%					H4→L1	16%
				H4→L2	4%					H3→L3	3%
				H3→L2	7%					H2→L3	5%
				H2→L3	29%						
S20	4.0874	303.34	0.0352	H7→L	2%						
				H5→L1	51%						
				H2→L3	41%						

AJ1-DPA						AJ1-TPA					
	eV	nm	f				eV	nm	f		
S1	2.3536	526.78	0.7249	H→L	98%	S1	2.2144	559.9	0.5073	H→L	95%
S2	2.5279	490.47	0.1107	H3→L	6%	S2	2.2921	540.92	0.2756	H1→L	99%
				H1→L	29%	S3	2.4527	505.51	0.5634	H3→L	5%
				H→L1	62%					H2→L1	4%
S3	2.6699	464.39	1.2175	H3→L	4%					H→L1	89%
				H1→L	69%	S4	2.5076	494.44	0.2706	H2→L	15%
				H→L1	25%					H1→L1	79%

State	Energy (eV)	λ (nm)	f	Transition	%
S4	2.7866	444.93	0.0251	H2→L	93%
				H2→L2	2%
S5	2.7968	443.31	0.7138	H3→L	87%
				H→L1	11%
S6	2.852	434.72	0.3095	H1→L1	88%
				H→L2	8%
S7	2.9074	426.45	0.0197	H1→L1	7%
				H→L2	89%
S8	2.9857	415.27	0.0002	H3→L1	89%
				H2→L	3%
				H2→L1	3%
S9	3.0372	408.22	0.0499	H3→L1	3%
				H2→L1	92%
S10	3.2093	386.33	0.0006	H3→L2	3%
				H1→L2	34%
				H→L3	59%
S11	3.2421	382.42	0.2229	H5→L	3%
				H4→L	90%
				H2→L2	2%
S12	3.2818	377.79	0.4484	H5→L	24%
				H4→L	2%
				H1→L2	46%
				H→L3	18%
S13	3.3108	374.49	0.0245	H6→L	15%
				H6→L2	2%
				H5→L	44%
				H5→L2	7%
				H4→L1	3%
				H1→L2	12%
				H→L3	10%
S14	3.4095	363.65	0.029	H4→L	3%

State	Energy (eV)	λ (nm)	f	Transition	%
				H→L	3%
S5	2.5413	487.88	0.1109	H2→L	79%
				H1→L1	17%
S6	2.6355	470.45	0.1326	H3→L	64%
				H2→L1	25%
				H→L1	9%
S7	2.8024	442.41	1.0889	H3→L	28%
				H2→L1	67%
S8	2.8219	439.36	0.0479	H2→L2	4%
				H→L2	92%
S9	2.8572	433.93	0.0195	H3→L1	97%
S10	2.906	426.65	0.0582	H1→L2	97%
S11	3.0871	401.62	0.2019	H4→L	36%
				H2→L2	58%
S12	3.1293	396.2	0.1565	H4→L	59%
				H2→L2	35%
				H→L2	3%
S13	3.1679	391.37	0.118	H6→L	3%
				H3→L2	2%
				H→L3	89%
S14	3.215	385.64	0.0185	H7→L	3%
				H6→L	73%
				H6→L2	8%
				H5→L	3%
				H→L3	4%
S15	3.2234	384.64	0.0111	H1→L3	96%
S16	3.2744	378.65	0.0027	H8→L	2%
				H5→L	15%
				H4→L1	68%
				H3→L2	11%
S17	3.3046	375.18	0.0484	H5→L	4%

State	eV	nm	f	Transition	%	State	eV	nm	f	Transition	%
				H3→L2	3%					H4→L1	7%
				H2→L2	88%					H3→L2	80%
S15	3.4122	363.36	0.0848	H4→L1	5%					H2→L3	2%
				H3→L2	84%					H→L3	2%
				H2→L2	3%	S18	3.3968	365	0.0353	H17→L	4%
				H→L3	4%					H7→L1	4%
S16	3.4426	360.15	0.0224	H6→L	27%					H6→L1	75%
				H5→L	3%					H6→L3	4%
				H5→L1	4%					H5→L1	2%
				H4→L1	57%	S19	3.4095	363.64	1.1517	H6→L	3%
S17	3.4837	355.9	0.0106	H12→L	2%					H6→L1	3%
				H6→L	3%					H5→L	65%
				H6→L1	14%					H4→L1	19%
				H5→L1	56%					H→L3	2%
				H5→L3	4%	S20	3.4761	356.67	0.0103	H8→L	2%
				H4→L1	3%					H3→L2	3%
				H1→L3	10%					H2→L3	87%
S18	3.5143	352.8	0.0037	H5→L1	7%						
				H1→L3	85%						
S19	3.6895	336.05	0.02	H3→L3	92%						
				H2→L3	3%						
S20	3.711	334.1	0.1059	H6→L	12%						
				H5→L	3%						
				H4→L1	11%						
				H3→L3	2%						
				H2→L3	65%						
				H→L3	3%						

AJ2-TPA						AJ2-DPA					
	eV	nm	f				eV	nm	f		
S1	1.9867	624.07	0.1895	H→L	98%	S1	1.8823	658.7	0.1743	H1→L1	2%

State	E (eV)	λ (nm)	f	Transition	%	State	E (eV)	λ (nm)	f	Transition	%
S2	2.0173	614.59	0.0725	H1→L	98%					H→L	96%
S3	2.2423	552.95	0.0289	H1→L1	97%	S2	1.9234	644.6	0.094	H1→L	98%
S4	2.2446	552.36	0.1925	H→L1	97%	S3	2.1261	583.15	0.1499	H1→L1	2%
S5	2.6244	472.44	0.0237	H→L2	95%					H→L1	95%
S6	2.6666	464.96	0.0003	H1→L2	97%	S4	2.1299	582.11	0.0168	H1→L1	93%
S7	2.7669	448.1	0.4596	H2→L	96%					H→L	3%
S8	2.8827	430.1	0.0034	H3→L	53%					H→L1	2%
				H2→L1	31%	S5	2.5473	486.72	0.0023	H→L2	96%
				H→L3	10%	S6	2.5847	479.68	0.0013	H1→L2	97%
S9	2.9466	420.77	0.1096	H2→L1	21%	S7	2.8201	439.64	0.6099	H2→L	97%
				H→L3	75%	S8	2.9014	427.32	0.0004	H3→L	3%
S10	2.9615	418.65	0.0008	H1→L3	97%					H→L3	93%
S11	2.9983	413.52	0.7782	H3→L	44%	S9	2.9272	423.55	0.0059	H1→L3	98%
				H2→L1	40%	S10	2.9363	422.25	0.2299	H5→L	3%
				H→L3	13%					H3→L	14%
S12	3.1478	393.87	0.0319	H4→L	21%					H2→L1	76%
				H3→L1	71%					H→L3	3%
				H2→L2	4%	S11	3.1172	397.74	0.9092	H3→L	79%
S13	3.1753	390.47	0.2611	H4→L	73%					H2→L1	16%
				H3→L1	23%	S12	3.2476	381.78	0.0682	H6→L	12%
S14	3.2452	382.05	0.0712	H11→L1	2%					H5→L	3%
				H6→L	55%					H4→L	51%
				H6→L2	9%					H3→L1	20%
				H5→L	28%					H2→L2	7%
				H5→L2	3%	S13	3.2711	379.03	0.0551	H6→L	53%
S15	3.3309	372.22	0.0279	H3→L1	2%					H6→L2	7%
				H2→L2	90%					H5→L	14%
S16	3.3726	367.63	0.0353	H6→L	6%					H4→L	5%
				H5→L	17%					H3→L1	11%
				H4→L1	70%					H2→L2	3%
				H2→L1	3%	S14	3.3087	374.72	0.0878	H4→L	34%

	eV	nm	f	Transition	%		eV	nm	f	Transition	%
S17	3.4342	361.03	0.0145	H11→L	5%					H3→L1	62%
				H11→L2	3%	S15	3.3702	367.88	0.0052	H6→L1	3%
				H6→L1	58%					H4→L	4%
				H6→L3	5%					H3→L1	4%
				H5→L1	22%					H2→L2	85%
				H2→L2	2%	S16	3.4519	359.17	0.1689	H15→L	3%
S18	3.4949	354.75	1.1396	H6→L	23%					H6→L	5%
				H5→L	46%					H6→L1	37%
				H4→L1	24%					H6→L3	2%
S19	3.5809	346.23	0.0104	H3→L2	90%					H5→L	22%
				H2→L3	6%					H5→L1	7%
S20	3.6731	337.55	0.0166	H10→L	4%					H4→L1	15%
				H3→L2	5%	S17	3.4618	358.15	0.3278	H15→L	2%
				H2→L3	84%					H6→L	8%
										H6→L1	29%
										H5→L	38%
										H5→L1	6%
										H4→L1	6%
						S18	3.5328	350.95	0.3182	H6→L	5%
										H5→L	13%
										H4→L1	73%
						S19	3.7001	335.08	0.1775	H9→L	26%
										H7→L	9%
										H6→L1	9%
										H5→L1	37%
										H1→L7	7%
						S20	3.7206	333.24	0.0233	H3→L2	40%
										H2→L3	50%

AJ2-TPA

eV	nm	f

S1	1.997	620.86	0.171	H→L	98%
S2	2.0205	613.63	0.0547	H1→L	99%
S3	2.2462	551.98	0.103	H→L1	97%
S4	2.2496	551.15	0.0265	H1→L1	97%
S5	2.5955	477.68	0.4061	H2→L	84%
				H→L2	12%
S6	2.6663	465.01	0.0304	H2→L	13%
				H→L2	85%
S7	2.6695	464.45	0.0053	H3→L	25%
				H2→L1	9%
				H1→L2	63%
S8	2.7071	457.99	0.0248	H3→L	54%
				H2→L1	8%
				H1→L2	34%
				H→L1	2%
S9	2.8398	436.6	0.8131	H3→L	17%
				H2→L1	78%
S10	2.9246	423.94	0.0178	H3→L1	91%
				H1→L3	5%
S11	2.9921	414.37	0.0031	H→L3	98%
S12	3.0043	412.69	0	H3→L1	5%
				H1→L3	93%
S13	3.0927	400.9	0.4822	H4→L	95%
S14	3.2012	387.31	0.0272	H2→L2	94%
S15	3.2536	381.06	0.001	H6→L	9%
				H5→L	27%
				H4→L1	58%
S16	3.2684	379.34	0.1012	H6→L	58%
				H6→L2	7%
				H5→L	5%
				H4→L1	24%

S17	3.3814	366.67	0.0417	H3→L2	93%
S18	3.4512	359.25	0.0669	H19→L	5%
				H19→L2	2%
				H6→L1	64%
				H6→L3	4%
				H5→L	4%
				H5→L1	13%
S19	3.4562	358.73	0.9721	H6→L	16%
				H6→L1	5%
				H5→L	50%
				H4→L1	11%
				H2→L3	4%
				H1→L5	4%
				H→L4	4%
S20	3.5799	346.33	0.0599	H18→L	2%
				H3→L2	2%
				H2→L3	87%