

Supplementary Information

Table S1. Experimental and Calculated Energy of Molecular Orbitals of **(III)** and Associated Transitions.

$\lambda_{\max}$ (nm/eV)	Experimental (MO Contributions)	f^*	$\lambda_{\max}$ (nm/eV)	Calculated (MO Contributions)
320/3.88	HOMO→LUMO	2.02	277/4.48	HOMO→LUMO
320/3.89	HOMO-1→LUMO	2.02	266/4.66	HOMO-1→LUMO
320/3.89	HOMO→LUMO+1	2.02	230/5.38	HOMO→LUMO+1
320/4.88	HOMO-1→LUMO+1	2.02	222/5.57	HOMO-1→LUMO+1
252/4.88	HOMO→LUMO+2	0.85	188/6.61	HOMO-1→LUMO+2
252/4.88	HOMO→LUMO+3	0.85	186/6.76	HOMO→LUMO+3
252/4.88	HOMO-1→LUMO+2	0.85	181/6.86	HOMO-1→LUMO+3

Notes: f^* , $f = 4.32 \times 10^{-9} \epsilon_{\max} \Delta\omega/2$ Frontier molecular orbitals from output in B3LYP G(d) calculation.

Table S2. Experimental and Calculated Energy of Molecular Orbitals of **(IV)** and Associated Transitions.

$\lambda_{\max}$ (nm/eV)	Experimental (MO Contributions)	f^*	$\lambda_{\max}$ (nm/eV)	Calculated (MO Contributions)
317/3.88	HOMO→LUMO	1.99	281/4.41	HOMO→LUMO
317/3.89	HOMO-1→LUMO	1.99	266/4.67	HOMO-1→LUMO
317/3.89	HOMO→LUMO+1	1.99	232/5.32	HOMO→LUMO+1
317/4.88	HOMO-1→LUMO+1	1.99	222/5.58	HOMO-1→LUMO+1
252/4.88	HOMO→LUMO+2	0.77	195/6.36	HOMO→LUMO+2
252/4.88	HOMO→LUMO+3	0.77	193/6.44	HOMO→LUMO+3
252/4.88	HOMO-1→LUMO+2	0.77	187/6.62	HOMO-1→LUMO+2

Notes: f^* , $f = 4.32 \times 10^{-9} \epsilon_{\max} \Delta\omega/2$ Frontier molecular orbitals from output in B3LYP G(d) calculation.

Table S3. Experimental and Calculated Energy of Molecular Orbitals of **(V)** and Associated Transitions.

$\lambda_{\max}$ (nm/eV)	Experimental (MO Contributions)	f^*	$\lambda_{\max}$ (nm/eV)	Calculated (MO Contributions)
318/3.88	HOMO→LUMO	1.90	262/4.73	HOMO→LUMO
318/3.89	HOMO-1→LUMO	1.90	246/5.04	HOMO-1→LUMO
318/3.89	HOMO→LUMO+1	1.90	220/5.63	HOMO→LUMO+1
318/4.88	HOMO-1→LUMO+1	1.90	209/5.93	HOMO-1→LUMO+1
253/4.88	HOMO→LUMO+2	0.72	181/6.84	HOMO→LUMO+2
253/4.88	HOMO→LUMO+3	0.72	174/7.14	HOMO-1→LUMO+2
253/4.88	HOMO-1→LUMO+2	0.72	162/7.63	HOMO→LUMO+3

Notes: f^* , $f = 4.32 \times 10^{-9} \epsilon_{\max} \Delta\omega/2$ Frontier molecular orbitals from output in B3LYP G(d) calculation.

Table S4. Experimental and Calculated Energy of Molecular Orbitals of **(VI)** and Associated Transitions.

λ_{max} (nm/eV)	Experimental (MO Contributions)	f^*	λ_{max} (nm/eV)	Calculated (MO Contributions)
319/3.88	HOMO→LUMO	1.95	280/4.42	HOMO→LUMO
319/3.89	HOMO-1→LUMO	1.95	267/4.64	HOMO-1→LUMO
319/3.89	HOMO→LUMO+1	1.95	232/5.34	HOMO→LUMO+1
319/4.88	HOMO-1→LUMO+1	1.95	223/5.56	HOMO-1→LUMO+1
253/4.88	HOMO→LUMO+2	0.74	193/6.41	HOMO→LUMO+2
253/4.88	HOMO→LUMO+3	0.74	188/6.59	HOMO→LUMO+3
253/4.88	HOMO-1→LUMO+2	0.74	187/6.63	HOMO-1→LUMO+2

Notes: f^* , $f = 4.32 \times 10^{-9} \varepsilon_{\text{max}} \Delta\omega/2$ Frontier molecular orbitals from output in B3LYP G(d) calculation.

Table S5. Experimental and Calculated Energy of Molecular Orbitals of **(VII)** and Associated Transitions.

λ_{max} (nm/eV)	Experimental (MO Contributions)	f^*	λ_{max} (nm/eV)	Calculated (MO Contributions)
316/3.88	HOMO→LUMO	1.90	280/4.43	HOMO→LUMO
316/3.89	HOMO-1→LUMO	1.90	266/4.67	HOMO-1→LUMO
316/3.89	HOMO→LUMO+1	1.90	233/5.31	HOMO→LUMO+1
316/4.88	HOMO-1→LUMO+1	1.90	223/5.55	HOMO-1→LUMO+1
252/4.88	HOMO→LUMO+2	0.71	205/6.05	HOMO→LUMO+2
252/4.88	HOMO→LUMO+3	0.71	198/6.26	HOMO→LUMO+3
252/4.88	HOMO-1→LUMO+2	0.71	197/6.28	HOMO-1→LUMO+2

Notes: f^* , $f = 4.32 \times 10^{-9} \varepsilon_{\text{max}} \Delta\omega/2$ Frontier molecular orbitals from output in B3LYP G(d) calculation.

Table S6. Experimental and Calculated Energy of Molecular Orbitals of **(VIII)** and Associated Transitions.

λ_{max} (nm/eV)	Experimental (MO Contributions)	f^*	λ_{max} (nm/eV)	Calculated (MO Contributions)
316/3.88	HOMO→LUMO	2.00	266/4.67	HOMO→LUMO
316/3.89	HOMO-1→LUMO	2.00	264/4.69	HOMO-1→LUMO
319/3.89	HOMO→LUMO+1	2.00	223/5.56	HOMO→LUMO+1
316/4.88	HOMO-1→LUMO+1	2.00	222/5.57	HOMO-1→LUMO+1
252/4.88	HOMO→LUMO+2	0.75	201/6.18	HOMO→LUMO+2
252/4.88	HOMO→LUMO+3	0.75	200/6.20	HOMO-1→LUMO+2
252/4.88	HOMO-1→LUMO+2	0.75	195/6.37	HOMO→LUMO+3

Notes: f^* , $f = 4.32 \times 10^{-9} \varepsilon_{\text{max}} \Delta\omega/2$ Frontier molecular orbitals from output in B3LYP G(d) calculation.