

## 间位取代卟啉及其锌卟啉的电子吸收光谱

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## Electronic Absorption Spectra of *Meso*-Substituted Porphyrins and Their Zinc Derivatives

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**Table S1 TD-DFT/PBE-calculated one-electron transition and oscillator strengths of free-based porphyrin 1**

NO <sub>2</sub> PP	Wavelength/nm	TD-DFT/PBE		Oscillator strength
		Excitation/eV	One-electron transition	
$Q_x^0$	629.8	1.97	H-1→L; H-1→L+5; H→L+1; H→L+4	0.017
$Q_y^0$	586.8	2.11	H→L+4; H-1→L; H-1→L+5;	0.051
$B$	477.1	2.60	H-2→L+2;	0.0077
$B$	459.3	2.70	H-3→L; H-3→L+5;	0.0092
$B$	458.3	2.71	H-3→L+1; H-3→L+4;	0.0047
$B$	438.3	2.83	H-3→L+4; H-1→L; H-1→L+5; H→L+4; H→L+9;	0.254
$B$	426.3	2.91	H-3→L+5; H-1→L+4;	0.043
$B$	412.4	3.01	H→L+8;	0.116
$B$	411.4	3.02	H-3→L+4; H→L+9;	
$B$	404.9	3.06	H-6→L+1; H-5→L+2; H-4→L+3;	0.006

H: HOMO; L: LUMO

**Table S2 TD-DFT/PBE-calculated one-electron transition and oscillator strengths of free-based porphyrin 2**

NH <sub>2</sub> PP	Wavelength/nm	TD-DFT/PBE		
		Excitation/eV	One-electron Transition	Oscillator strength
$Q_x^0$	665.1	1.89	H-1→L+1; H-4→L; H→L;	0.028
$Q_y^0$	560.1	2.21	H-5→L+1; H-4→L; H→L;	0.016
$B$	444.5	2.79	H-9→L; H-7→L+1; H-5→L; H-4→L+1; H→L+1;	0.171
$B$	440.1	2.82	H-7→L; H-5→L+1;	0.023
$B$	409.4	3.04	H-11→L; H-9→L+1; H-7→L; H-5→L+1; H-4→L; H→L;	
$B$	408.7	3.03	H-11→L+2; H-9→L; H-7→L+1; H-5→L; H-3→L+1;	0.247

H: HOMO; L: LUMO

**Table S3 TD-DFT/PBE-calculated one-electron transition and oscillator strengths of free-based porphyrin 3**

NO <sub>2</sub> ZnPP	Wavelength/nm	TD-DFT/PBE		
		Excitation/eV	One-electron transition	Oscillator Strength
<i>Q</i> <sup>0</sup>	582.9	2.13	H-1→L+5; H→L+4;	0.029
<i>B</i>	443.8	2.79	H-4→L; H-3→L+2;	0.003
<i>B</i>	443.2	2.80	H-4→L+1; H-3→L+3;	0.007
<i>B</i>	442.4	2.81	H-4→L+3;	0.004
<i>B</i>	442.3	2.81	H-5→L;	0.006
<i>B</i>	416.4	2.98	H-1→L+5; H→L+4; H→L+9;	0.673

H: HOMO; L: LUMO

**Table S4 TD-DFT/PBE-calculated one-electron transition and oscillator strengths of free-based porphyrin 4**

NH <sub>2</sub> ZnPP	TD-DFT/PBE			
	Wavelength/nm	Excitation/eV	One-electron Transition	Oscillator Strength
<i>Q</i> <sup>0</sup>	637.1	1.95	H-5→L; H-4→L+1; H→L+1;	0.023
<i>Q</i> <sup>0</sup>	563.0	2.20	H-6→L; H-5→L+1; H-4→L; H→L;	0.017
<i>B</i>	505.9	2.45	H-6→L; H-5→L+1;	0.004
<i>B</i>	415.2	2.99	H-13→L; H-11→L+1; H-8→L; H-5→L+1; H-4→L; H-3→L+2; H→L;	0.508
<i>B</i>	411.7	3.01	H-13→L+1; H-11→L; H-5→L;	0.052
<i>B</i>	397.1	3.12	H-13→L+1; H-11→L; H-5→L;	0.013

H: HOMO; L: LUMO