Impact of tert-butyl on mechanofluorochromism of triaryl-substituted phenothiazine derivatives

He Zhao, Siwen Hu, Meng Liang, Pengchong Xue*

Tianjin Key Laboratory of Structure and Performance for Functional Molecules, College of Chemistry, Tianjin Normal University, No. 393, Binshui West Road, Tianjin, 300387, P. R. China. Email: xuepengchong@126.com; hxxyxpc@tjnu.edu.cn

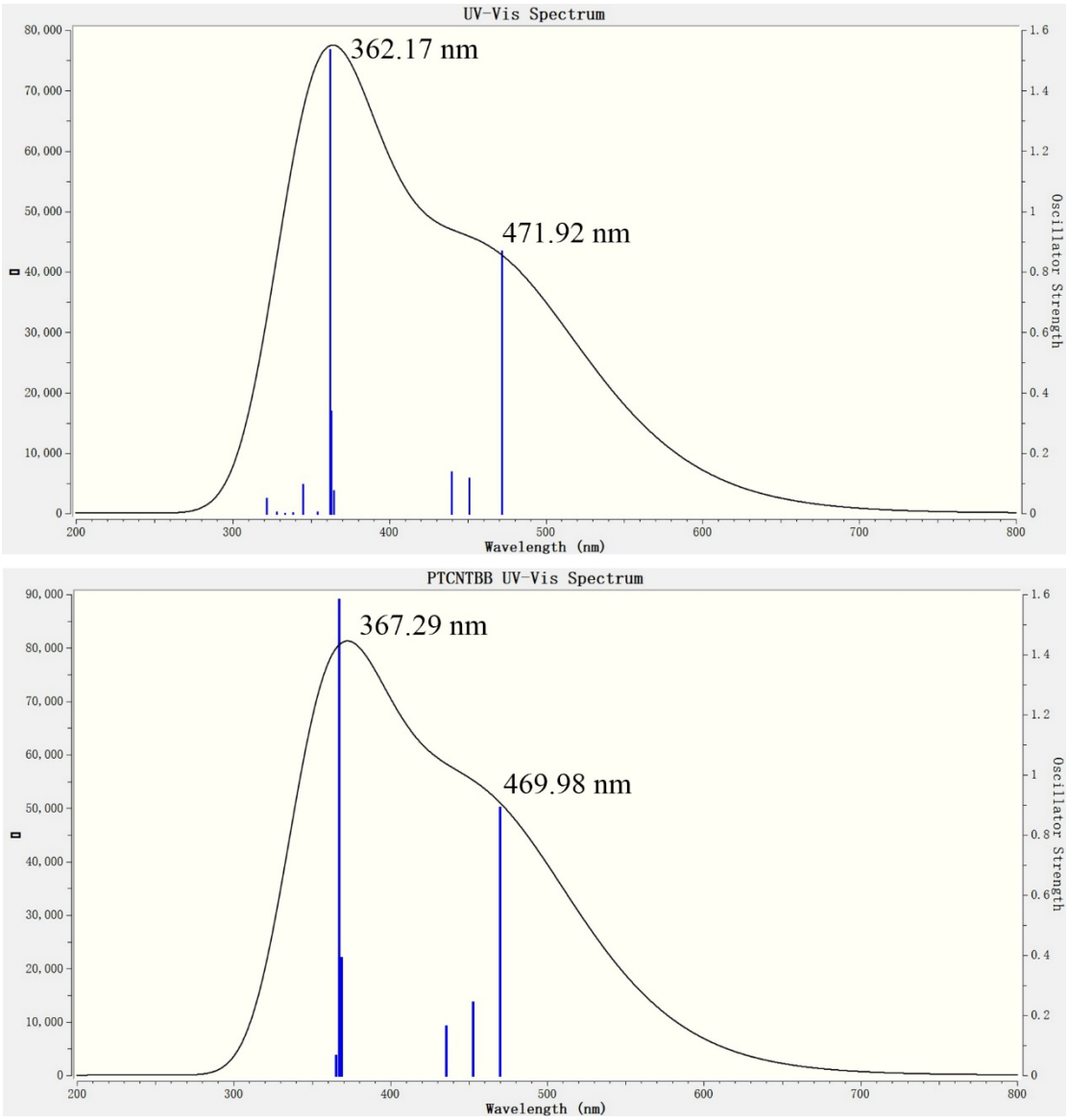

Figure S1. Simulated absorption spectra of (top) PTCNB and (bottom) PTCNTBB.

Table S1. Energy levels of frontier orbitals and date of corresponding electron transitions.

	E_{HOMO} (eV)	E_{LUMO} (eV)	Dipole moment (D)	Assignment of transition	λ_{ab} (nm)	Energy (eV)	oscillator strength
PTCNB	-5.59	-2.58	7.70	H-2→L (38.5 %) H-1→L+1 (49.0 %)	362.17	3.4167	1.5352
				H→L (90.6 %) H→L+2 (7.2 %)	471.92	2.6272	0.8689
PTCNTBB	-5.54	-2.51	8.48	H→L (83.9 %) H→L+2 (13.5 %)	367.29	3.3757	1.5821
				H-2→L (36.7 %) H-1→L+1 (58.0 %)	469.98	2.6381	0.8893

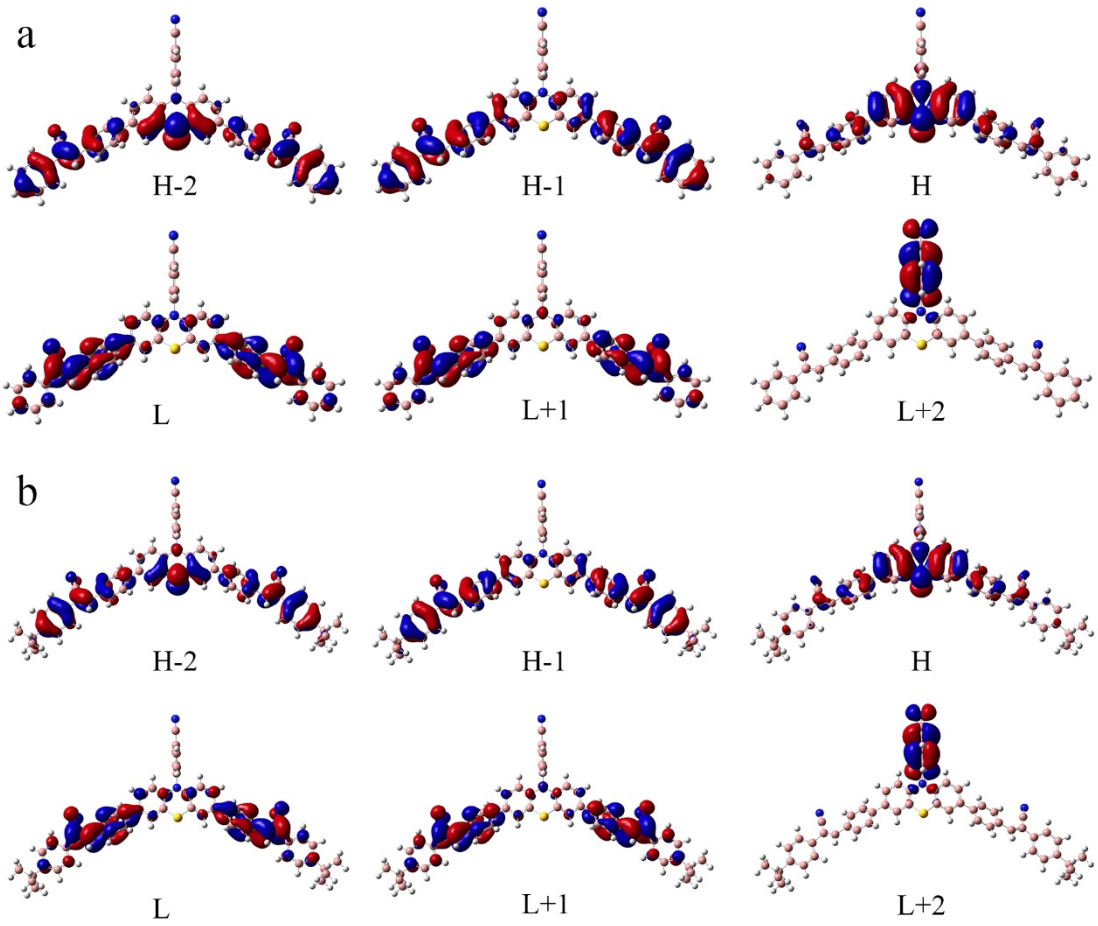

Figure S2. Frontier orbitals of (a) PTCNB and (b) PTCNTBB.

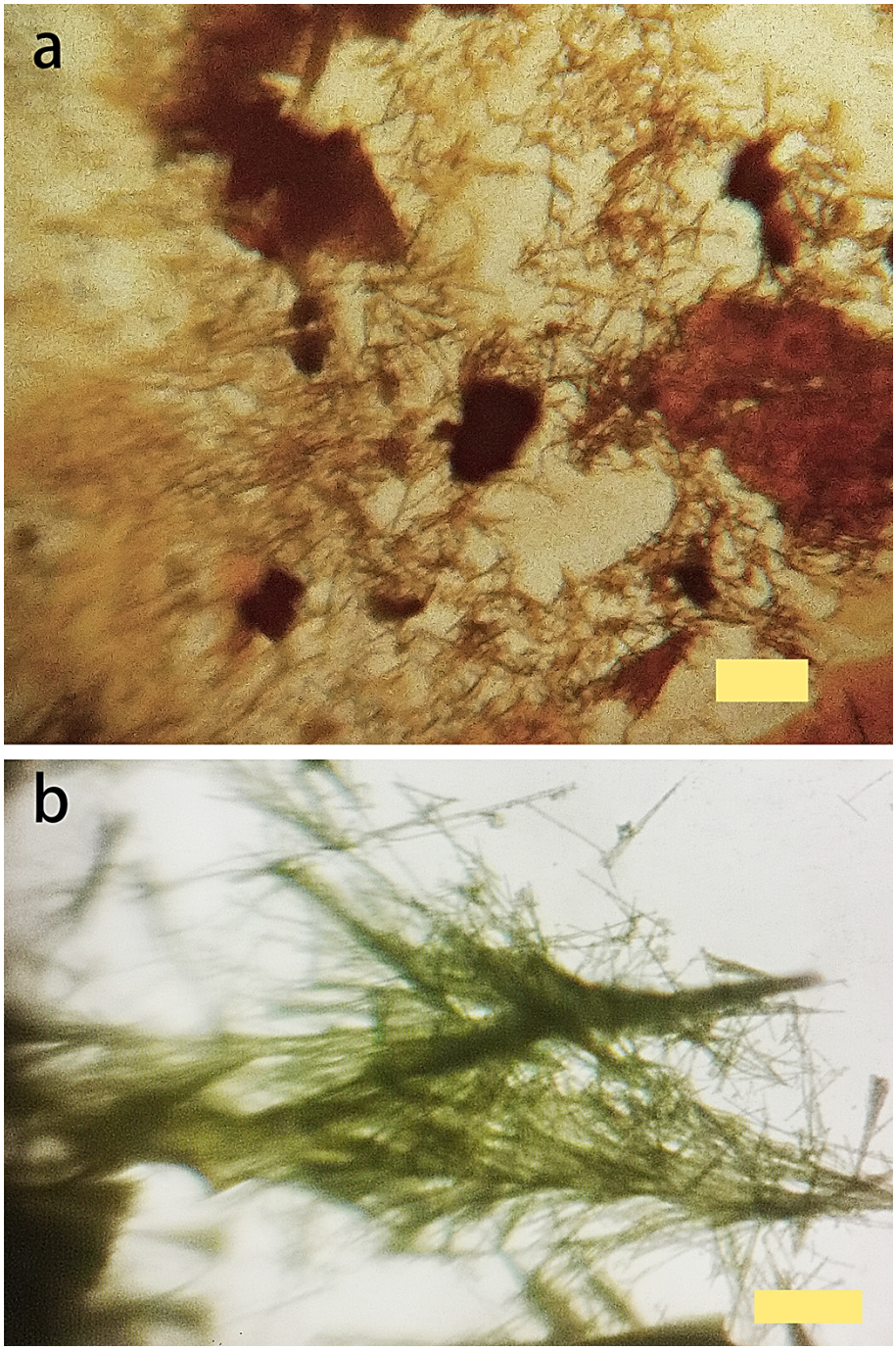

Figure S3. Optical microscopic images of (a) PTCNB and (b) PTCNTBB crystals from DCM/ethanol. Bar is 50 μm.

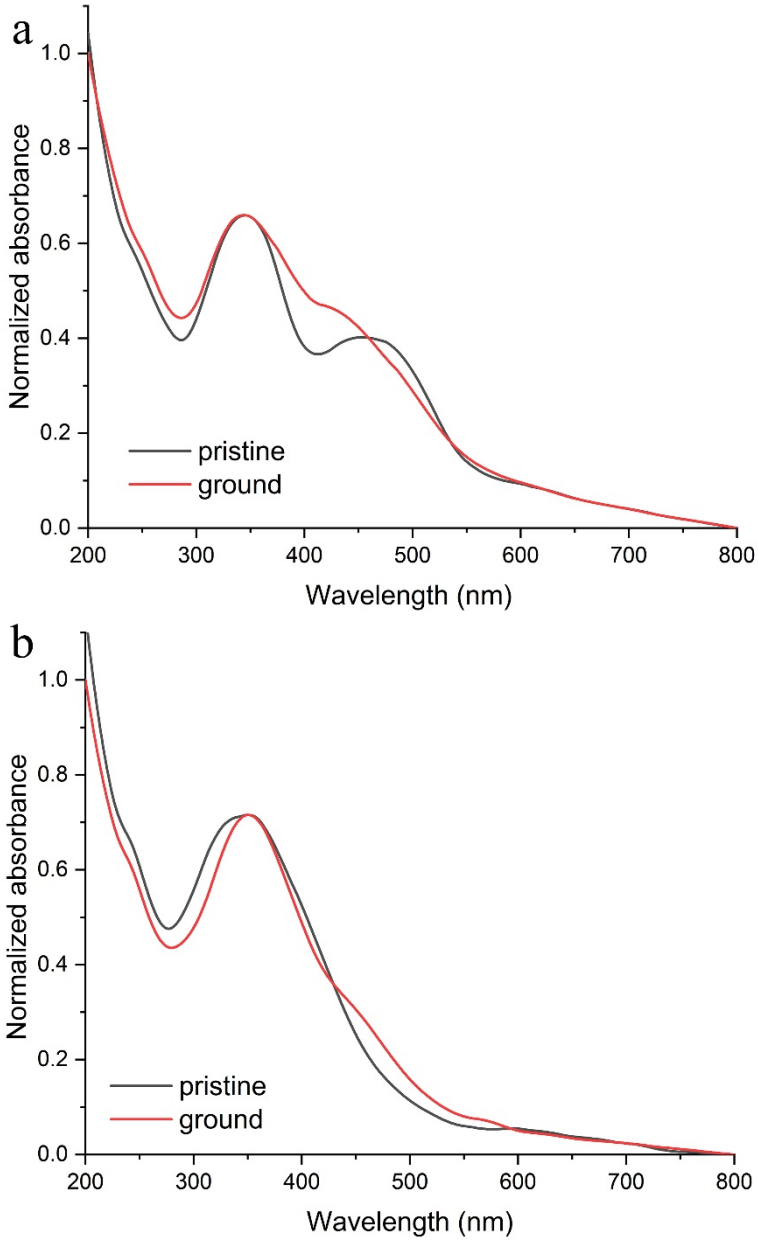

Figure S4. Normalized absorption spectra of (a) PTCNB and (b) PTCNTBB in pristine and ground states.