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Supporting information for

Phenothiazine-Based Benzoxazole Derivates Exhibiting Mechanochromic Luminescence: Effect of Bromine Atom

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Table S1 Electronic transition data obtained by the TD/DFT-B3LYP/6-31G calculation for **PVB** and **BPVB**.

	Electronic transition	λ_{abs} (nm)	E (eV)	Oscillator strength	Transition assignment
PVB	1	433.82	2.8580	0.4620	HOMO→ LUMO
BPVB	1	424.43	2.9212	0.6417	HOMO→ LUMO

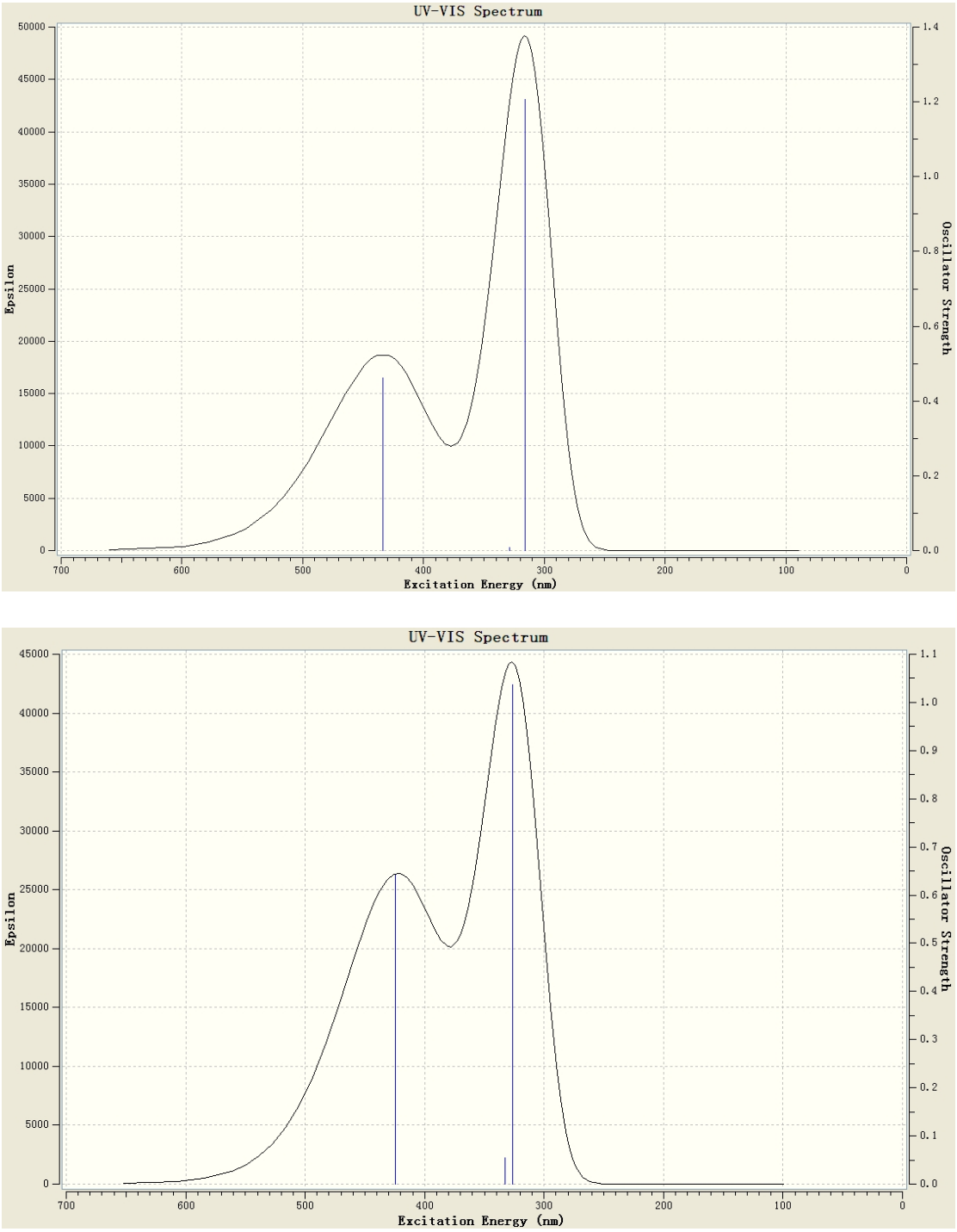

Fig. S1 Simulated UV-Vis absorption spectrum of **PVB** (top) and **BPVB** (bottom).

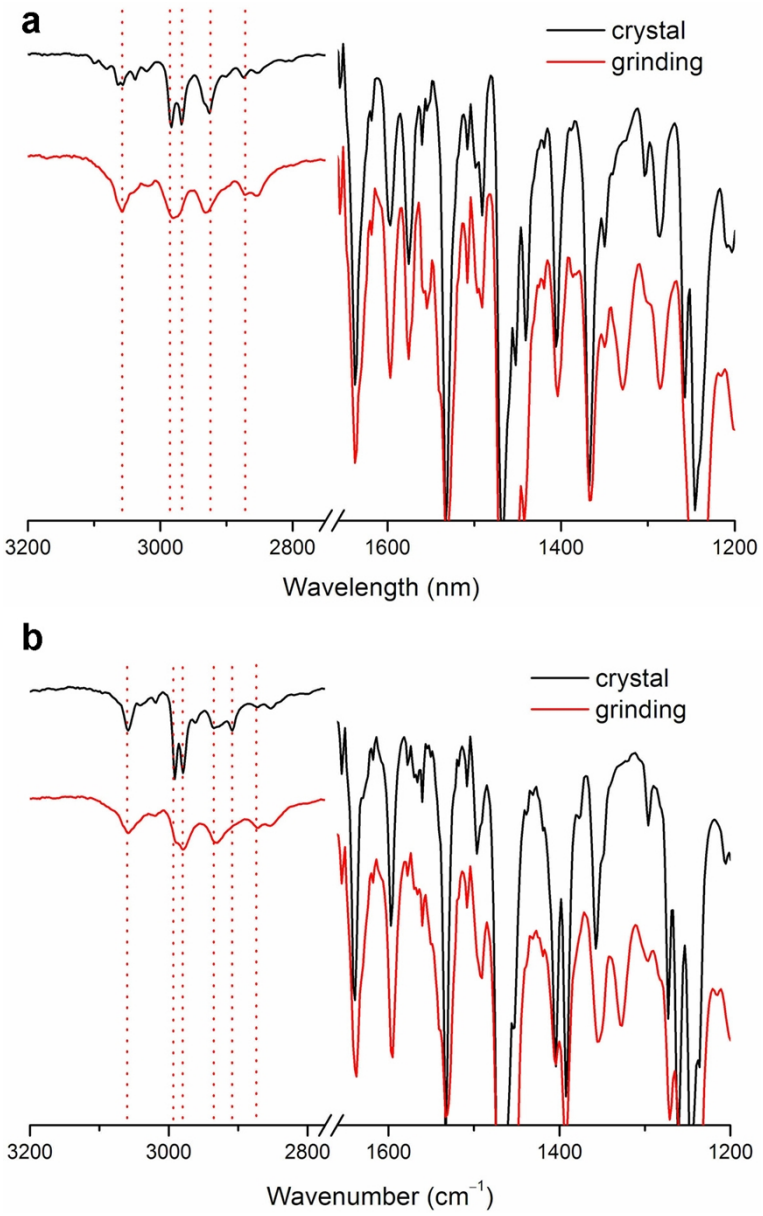

Fig. S2 IR spectra of **PVB** (a) and **BPVB** (b) before and after grinding.

Table S2. Crystal data of **PVB** and **BPVB**.

	PVB	**BPVB**
Formula sum	$C_{23}H_{18}N_2OS$	$C_{23}H_{16}BrN_2OS$
Formula weight	370.45	448.35
Crystal system	monoclinic	triclinic
Space group	*P* 21/c	*P* -1
Unit cell dimensions	*a* = 13.690(3) Å	*a* = 4.1159(8) Å
	b = 21.558(4) Å	*b* = 11.407(2) Å
	c = 6.2444(12) Å	*c* = 20.162(4) Å
	□ = 95.33(3) °	□ = 93.04(3) °
		□ = 91.76(3) °
		□ = 99.00(3) °
Cell volume	1834.94(60) $Å^3$	932.91(30) $Å^3$
Z	4	2
Density, calculated	1.341 g/cm^3	1.596 g/cm^3
R_{All}	0.076	0.076
Pearson code	mP180	aP88
Formula type	NOP2Q18R23	NOPQ2R23...
Wyckoff sequence	e^{45}	i^{44}

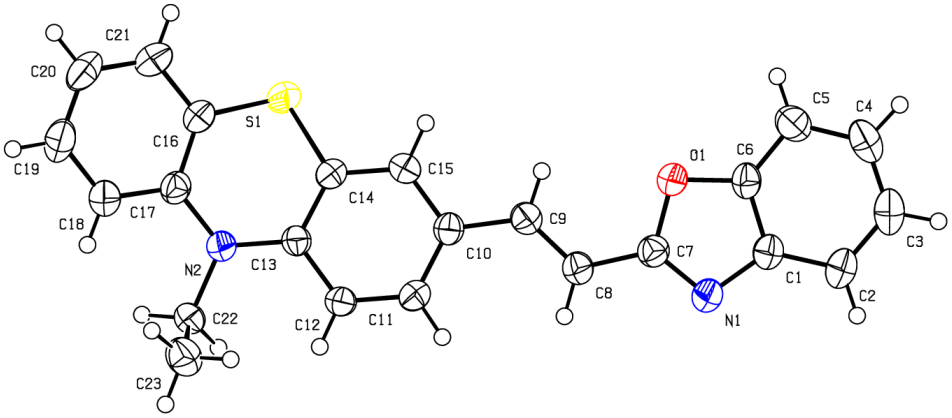

Fig. S3 Crystal structure of **PVB** (50% probability for thermal ellipsoids).

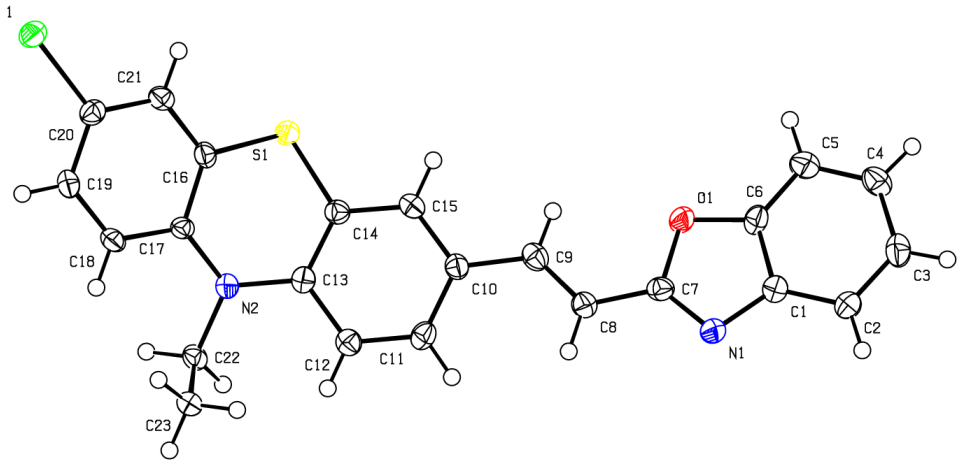

Fig. S4 Crystal structure of **BPVB** (50% probability for thermal ellipsoids).