

Electronic Supplementary Information

5-(2,6-Bis((E)-4-(dimethylamino)styryl)-1-ethylpyridin-4(1H)-ylidene)-2,2-dimethyl-1,3-dioxane-4,6-dione: aggregation-induced emission, polymorphism, mechanochromism, and thermochromism

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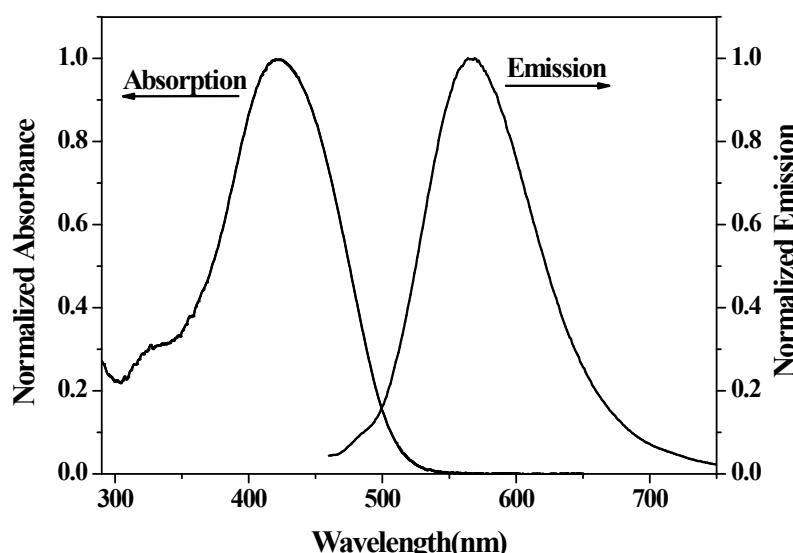


Fig. S1 UV-vis absorption and emission spectra of **DHPM** in DMSO solution (1×10^{-5} M).

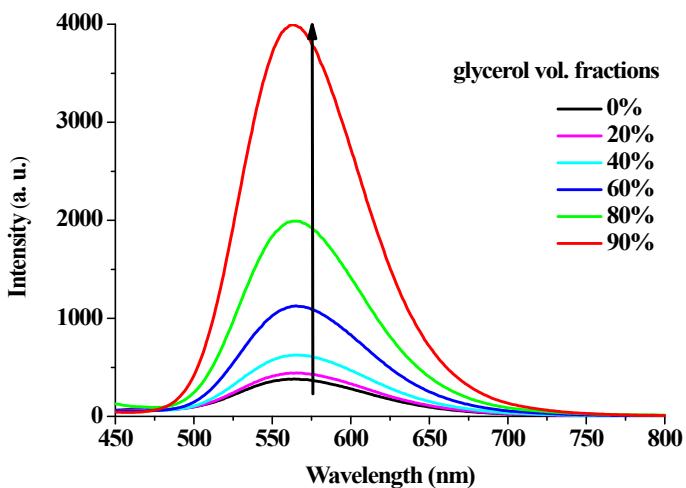


Fig. S2 Fluorescence spectra of **DHPM** in methanol/glycerol mixtures (1×10^{-5} M) with different glycerol volume fractions.

Table S1 Crystal data and details of collection and refinement for **DHPM-y**, **DHPM-o**, and **DHPM-r**.

	DHPM-y	DHPM-o	DHPM-r
Empirical formula	C ₃₃ H ₃₇ N ₃ O ₄	C ₇₂ H ₈₆ N ₃ O ₄	C ₃₃ H ₃₇ N ₃ O ₄
Formula weight	539.65	1163.46	539.65
Temperature (K)	296	293(2)	130
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	P12 ₁ /c1	P $\bar{1}$	P12 ₁ /c1
Z	4	2	4
D _{calcd} [Mg/m ³]	1.208	1.204	1.243
F (000)	1152	1248	1152
θ range [°]	3.527-66.666	1.476-24.998	1.655-27.506
R ₁ [I>2σ(I)]	0.0645	0.0666	0.0460
wR ₂ [I>2σ(I)]	0.1599	0.1672	0.0974
a [Å]	11.3869(7)	14.7343(14)	11.2361(14)
b [Å]	25.0608(16)	14.7727(15)	24.602(3)
c [Å]	10.4964(8)	15.7694(15)	10.5445(14)
α [deg]	90	92.545(3)	90
β [deg]	97.701(5)	93.186(2)	98.262(2)
γ [deg]	90	110.150(2)	90
V [Å ³]	2968.3(3)	3210.0(5)	2884.6(6)
GOF	1.032	0.982	0.975
R(int)	0.0876	0.0395	0.0587
No. of reflcns collected	26507	17908	23416
No. of unique reflcns	5096	11282	6623
R ₁ (all data)	0.0955	0.1284	0.0955
wR ₂ (all data)	0.1883	0.2063	0.1150

2. Spectra of NMR

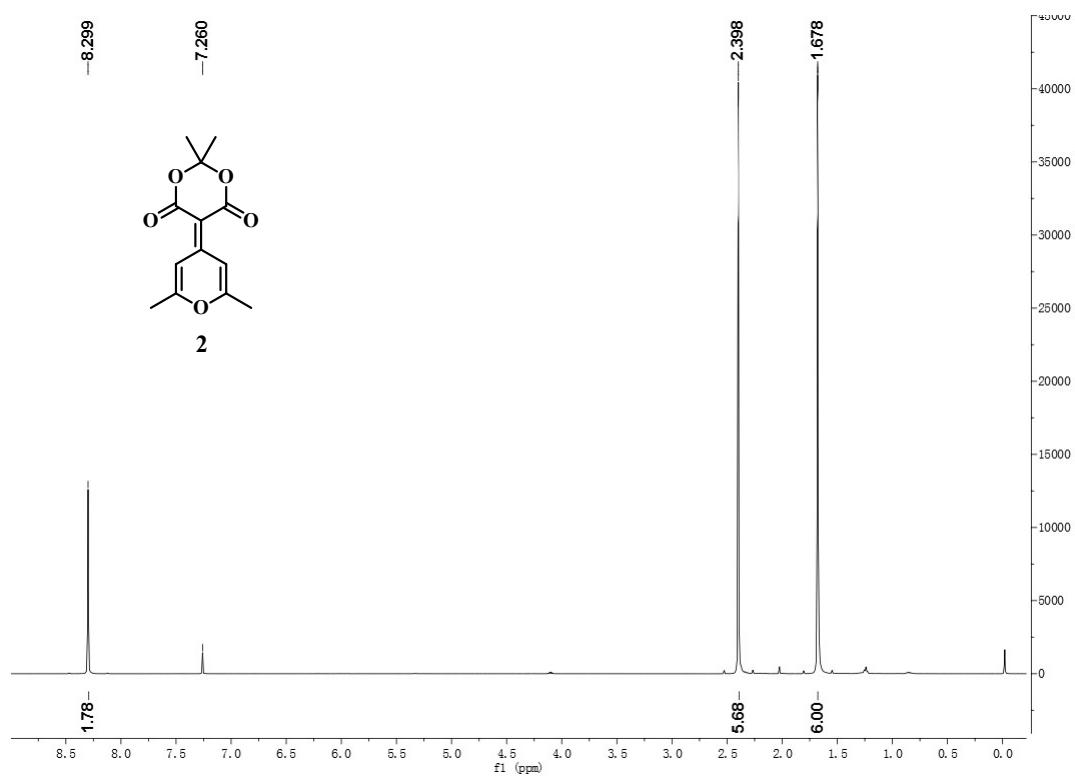


Fig. S3 ¹H NMR of compound 2 (CDCl₃, 500 MHz).

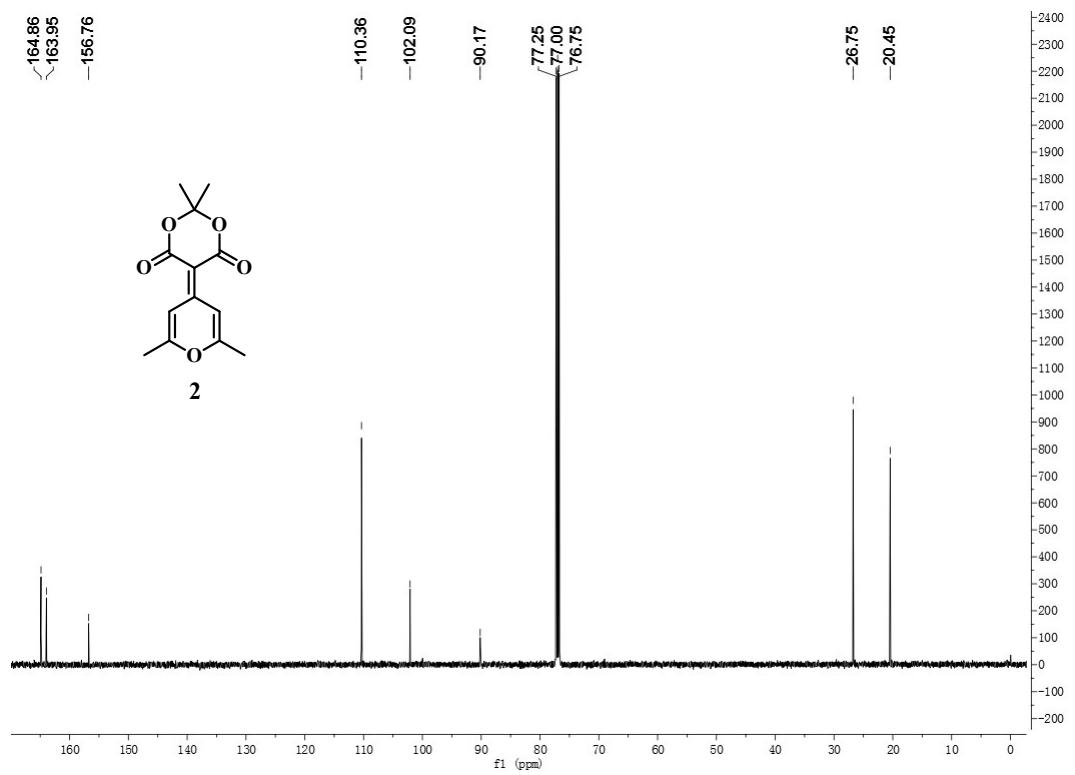


Fig. S4 ¹³C NMR of compound 2 (CDCl₃, 125 MHz).

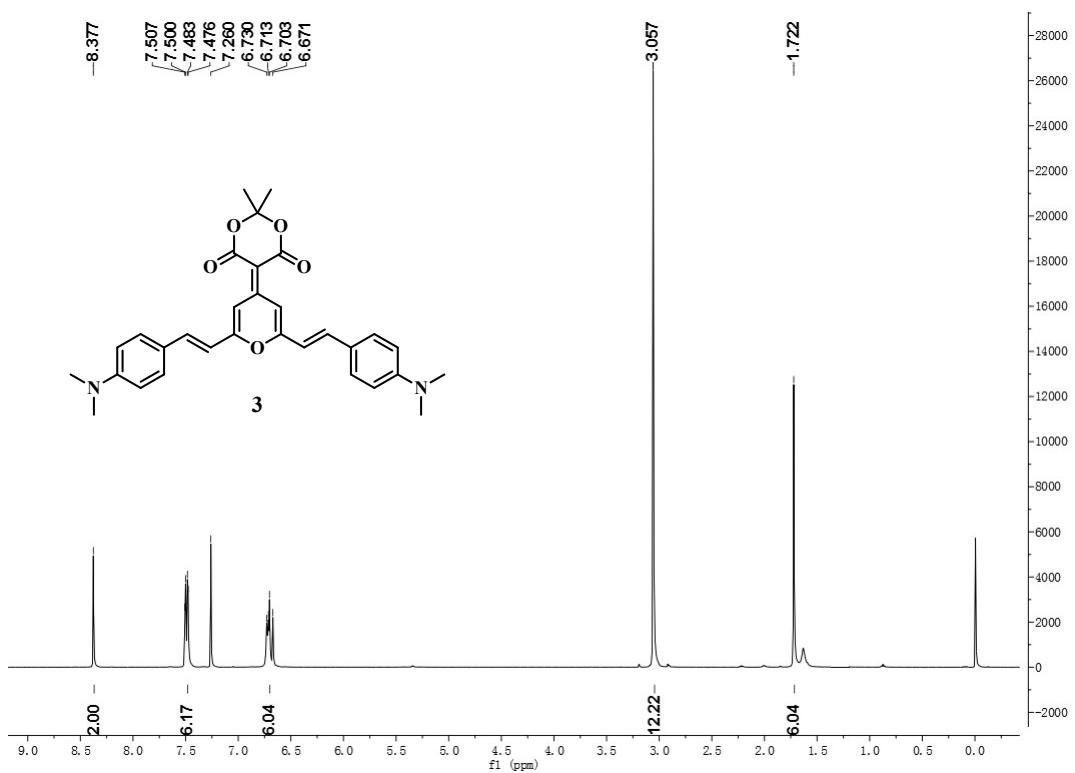


Fig. S5 ^1H NMR of compound **3** (CDCl_3 , 500 MHz).

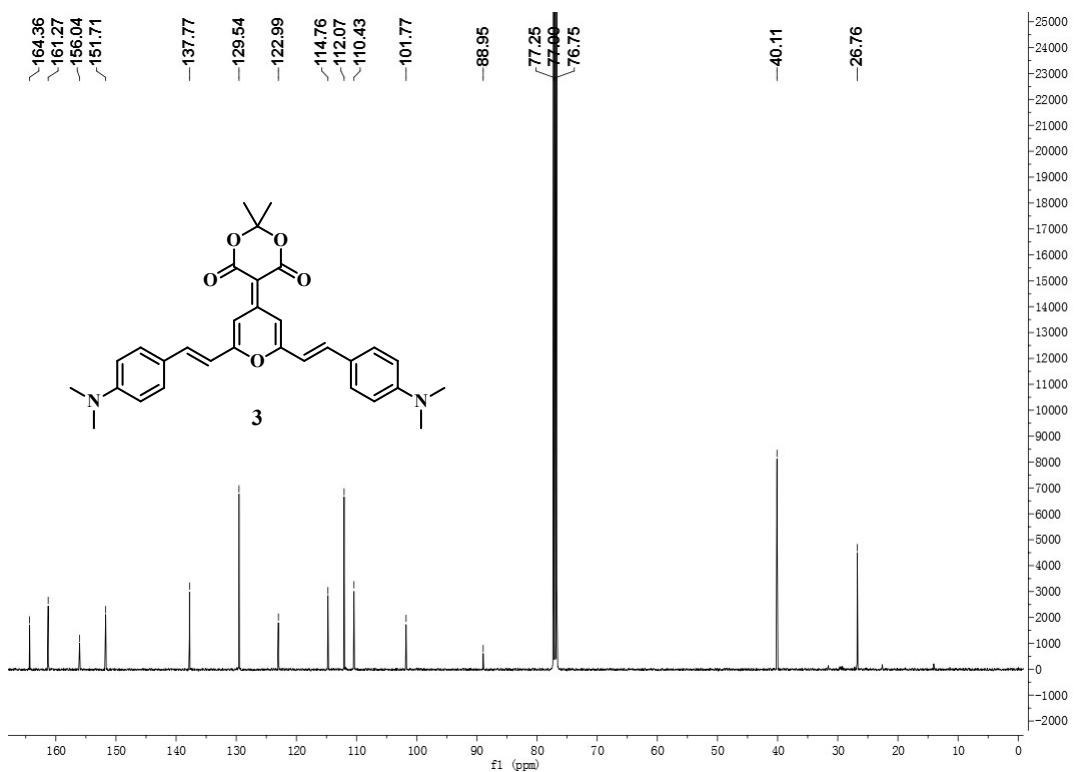


Fig. S6 ^{13}C NMR of compound **3** (CDCl_3 , 125 MHz).

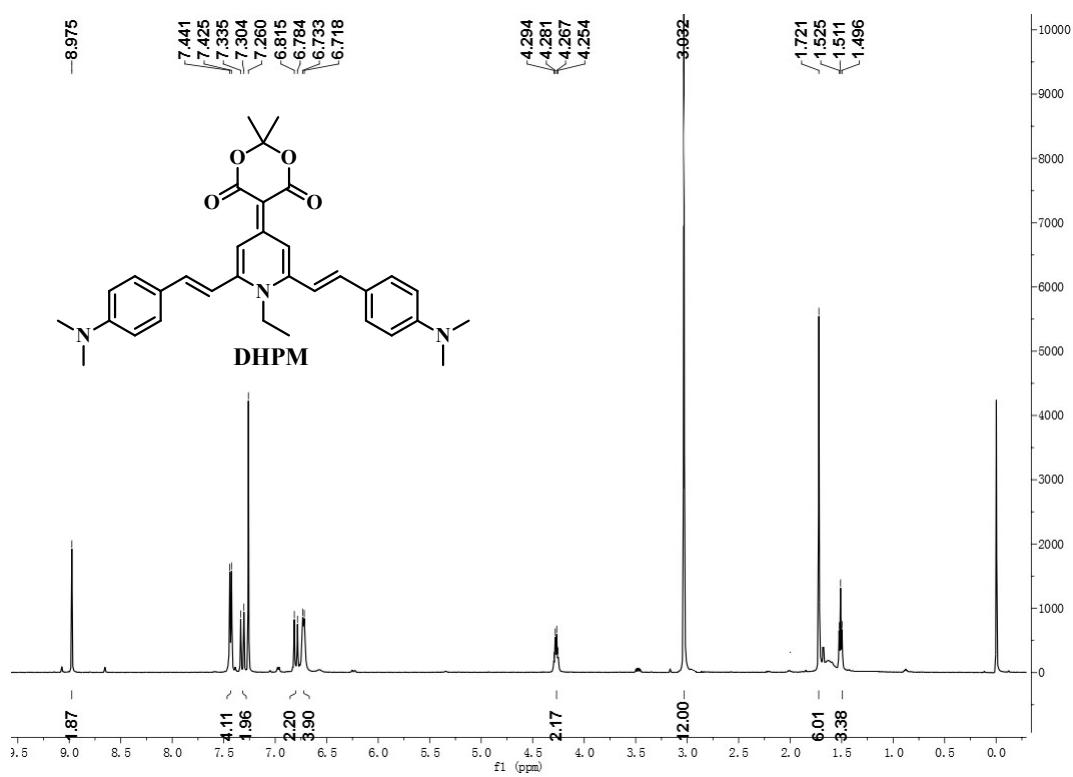


Fig. S7 ^1H NMR of **DHPM** (CDCl_3 , 500 MHz).

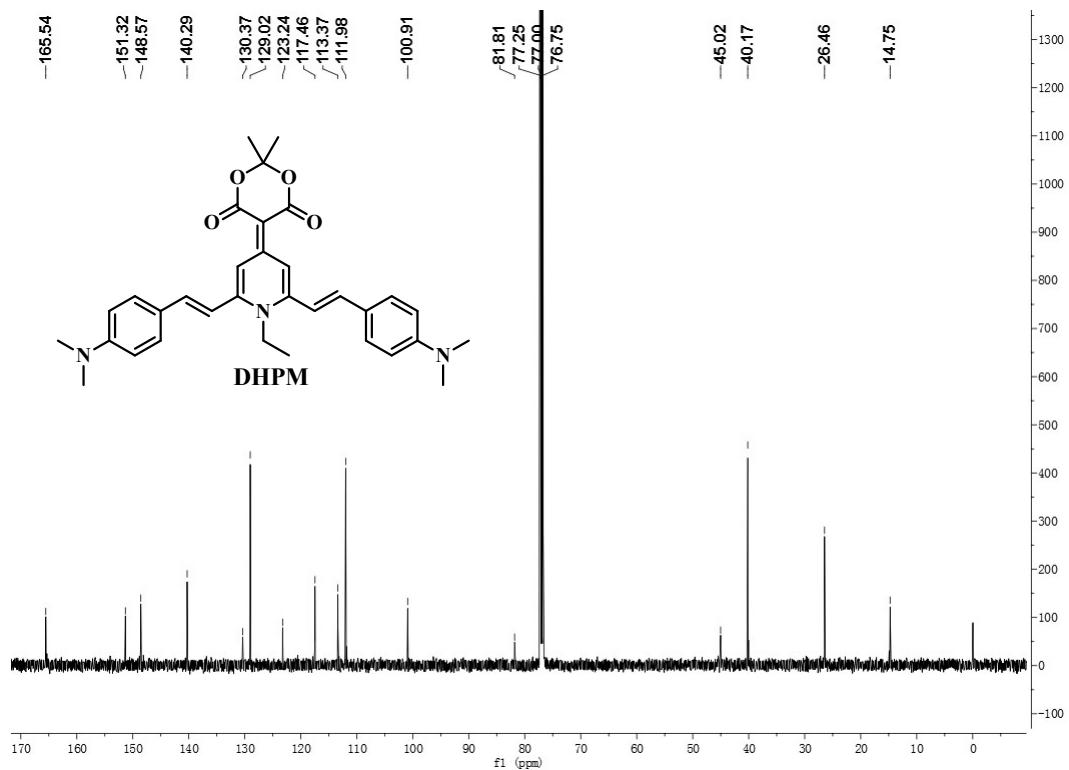


Fig. S8 ^{13}C NMR of **DHPM** (CDCl_3 , 125 MHz).