Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Luminescent Switching and Structural Transition through Multiple External Stimuli Based on Organic Molecular Polymorphs

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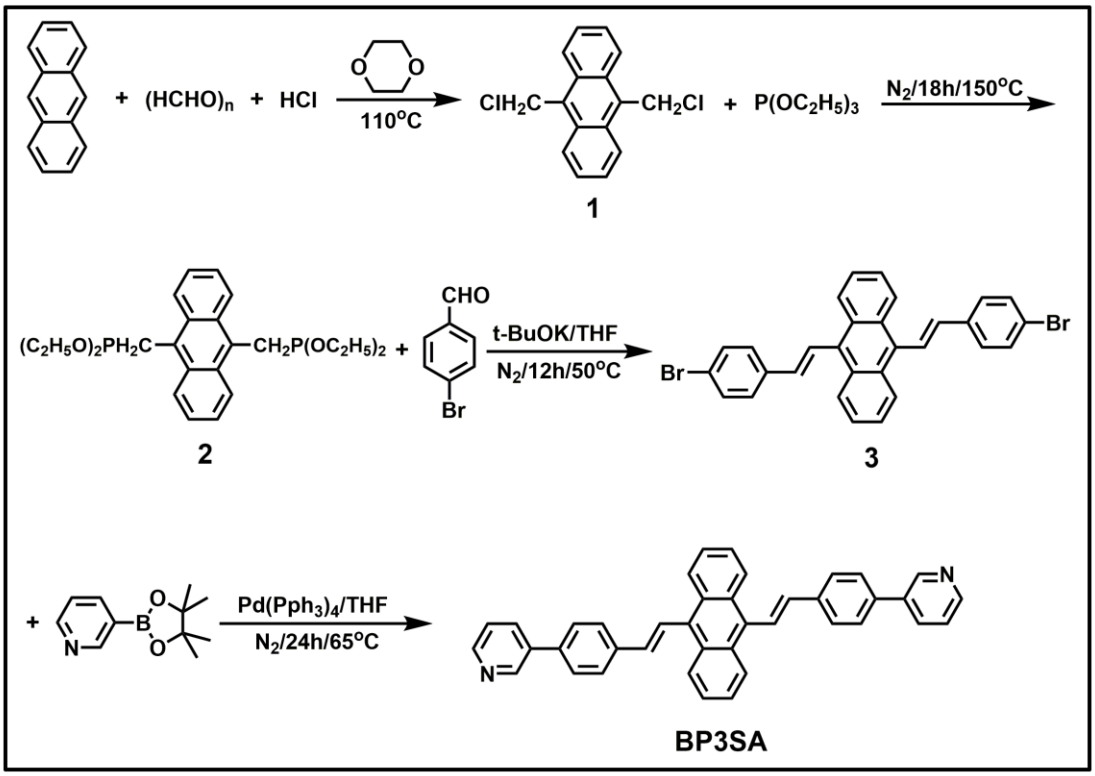

Scheme S1 Synthetic routes for BP3SA.

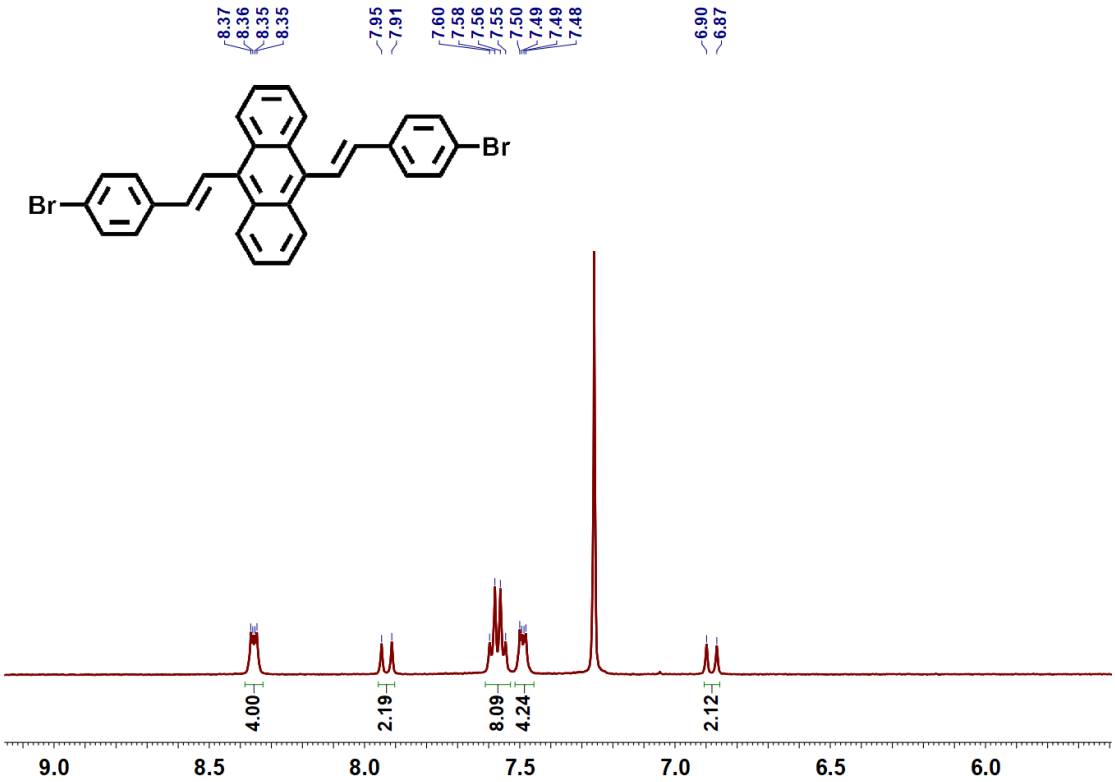

Fig. S1 [1]HNMR of Compound **3**.

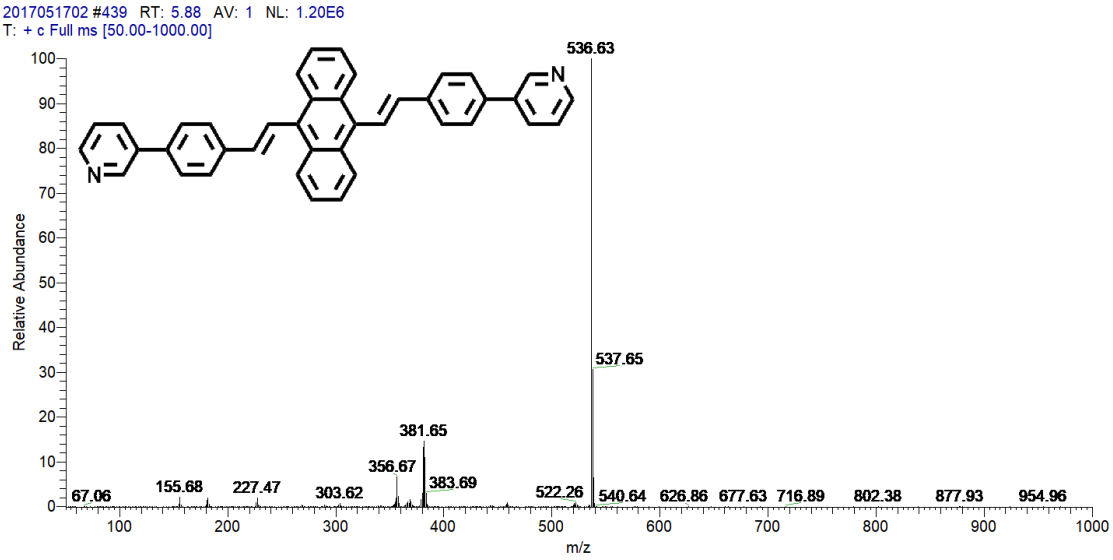

Fig. S2 MS of BP3SA.

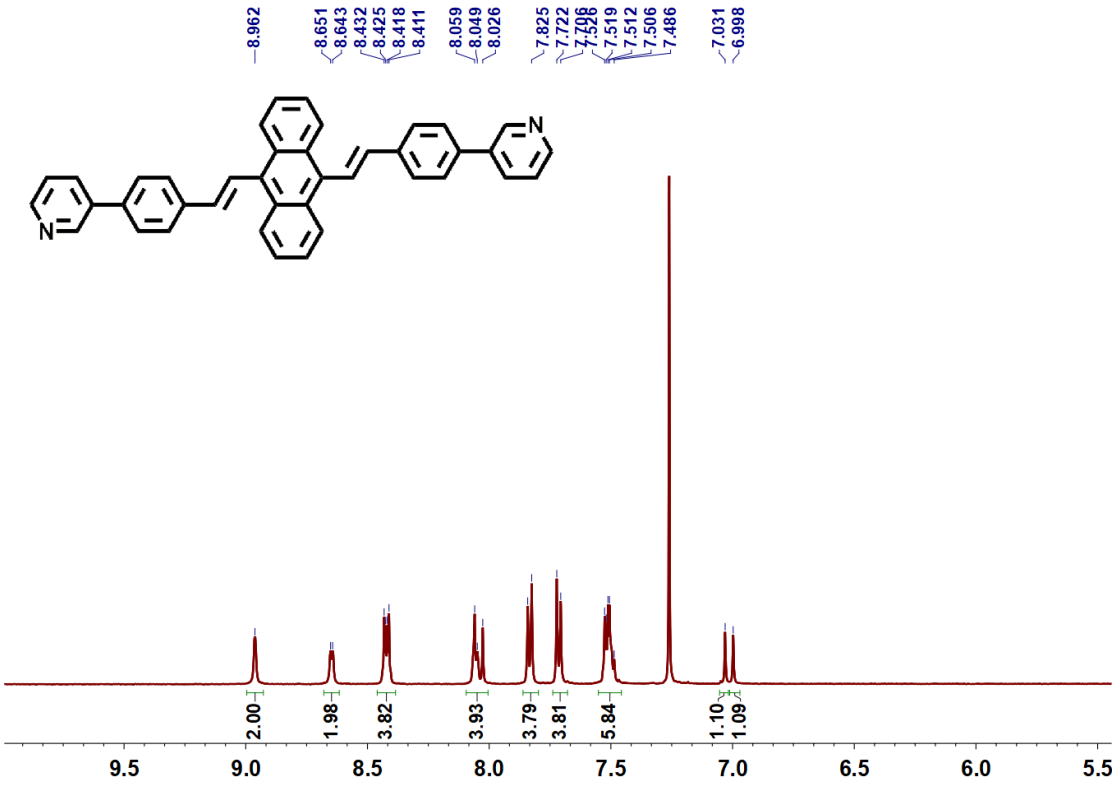

Fig S3. [1]HNMR of BP3SA.

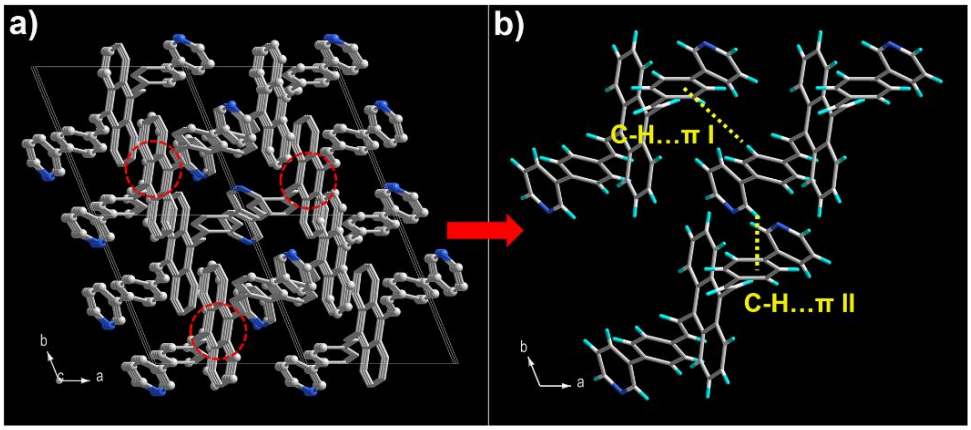

Fig. S4 a) The perspective view of G-phase cells along the c-axis. b) the intermolecular interactions C-H…π between adjacent molecules in G-phase.

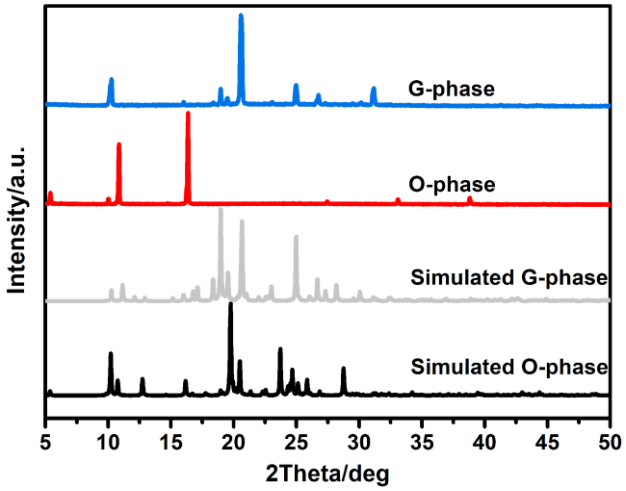

Fig. S5 PXRD patterns of G-phase and O-phase and simulated PXRD patterns obtained from the data of single crystals

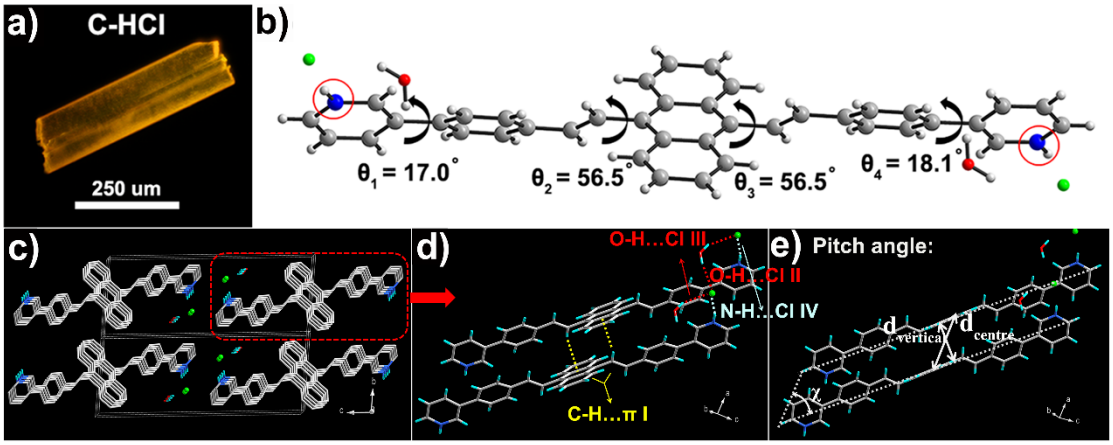

Fig. S6 Image (a) and molecular conformation (b) of C-HCl. (c) The perspective view of C-HCl cell along the c-axis. (d) the intermolecular interactions between adjacent molecules in C-HCl. (e) The vertical distance, the center distance and the pitch angle in C-HCl ($d_{vertical}$ = 3.421 Å, d_{centre} = 4.969 Å, χ = 45.4°).

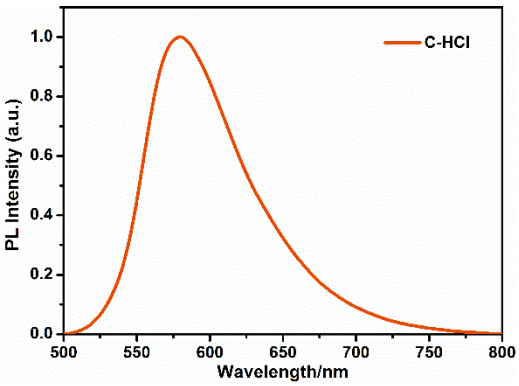

Fig. S7 Normalized PL spectra of C-HCl.

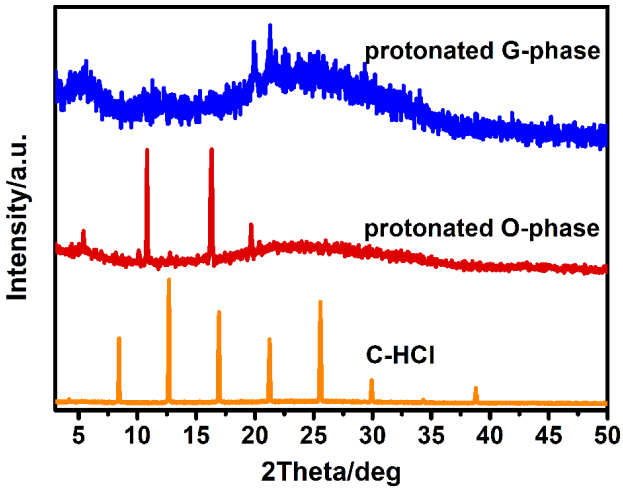

Fig. S8 PXRD patterns of protonated G-phase, protonated O-phase and C-HCl.

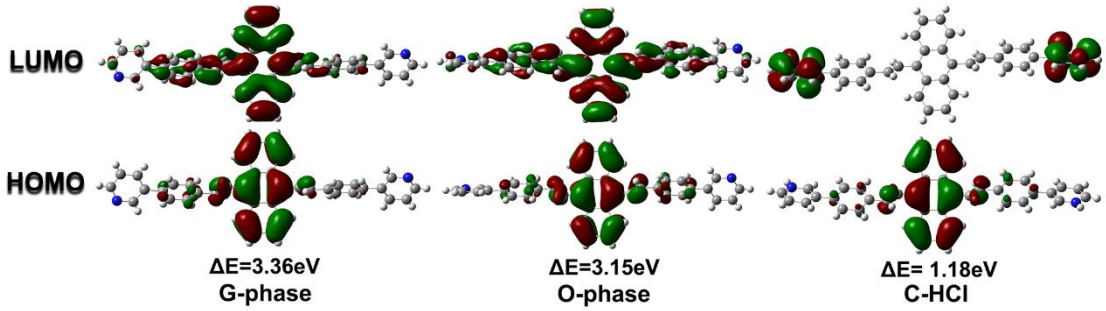

Fig. S9 Diagram of theoretical calculated frontier orbital contribution based on B3LYP-6-31G** of G-phase, O-phase and C-HCl.

Table S1 Photophysical data of BP3SA under different states.

State	λ_{em}	PLQY	τ /ns	k_{nr}	k_r
In THF	638	0.19	1.96	$4.13*10^8$	$9.69*10^7$
Powder	509	0.55	1.59	$2.83*10^8$	$3.46*10^8$
G-phase	511	0.98	1.40	$1.42*10^7$	$7.00*10^8$
O-phase	575	0.48	0.04	$1.30*10^{10}$	$1.20*10^{10}$

Table S2 Summary of intermolecular interactions in G-phase.

Orientation of interaction	*d*(Å)	*A*(deg)
C-H···π I	3.68	143.3
C-H···π II	2.85	130.2
C-H···π III	3.35	150.5
C-H···π IV	3.15	150.3
C-H···N V	3.48	174.2
C-H···N VI	3.02	143.3
C-H···N VII	3.34	141.0

Table S3 Summary of intermolecular interactions in O-phase.

Orientation of interaction	*d*(Å)	*A*(deg)
π···π I	3.75	
C-H···π II	2.85	130.2
C-H···π III	3.35	150.5
C-H···π IV	3.15	150.3
C-H···π V	3.48	174.2

Table S4 Summary of intermolecular interactions in C-HCl.

Orientation of interaction	*d*(Å)	*A*(deg)
C-H···π I	2.69	142.4
O-H···Cl II	2.48	166.1
O-H···Cl III	2.44	153.3
N-H···Cl IV	2.21	168.6

Table S5 Crystal data and structure refinements of G-phase, O-phase and C-HCl crystals.

	G-phase	O-phase	C-HCl
CCDC	1581638	1581639	1581640
Sum formula	$C_{40}H_{28}N_2$	$C_{40}H_{28}N_2$	$C_{40}H_{34}N_2O_2Cl_2$
formula wt	536.64	536.64	645.59
T, K	293 K	293 K	293 K
crystal system	triclinic	monoclinic	triclinic
space group	P -1	P 21/c	P -1
a, Å	9.4994(3)	9.3582(19)	4.9686(2)
b, Å	9.8382(3)	32.856(7)	8.1389(4)
c, Å	16.5464(5)	9.3637(19)	20.8828(10)

α, deg	95.704(1)	90	94.934(2)
β, deg	102.599(1)	106.42(3)	91.571(2)
γ, deg	110.032(1)	90	98.421(2)
V, Å3	1392.04(7)	2761.7(11)	831.59(7)
Z	2	4	1
density, g/cm3	1.280	1.291	1.289
M (Mo Kα), mm-1	0.074	0.574	2.051
θ range, deg	2.97–27.50	2.69–38.253	2.125–68.439
no. of reflcns collected	30869	23226	14982
no. of unique reflcns	6359	4944	2982
R(int)	0.0835	0.0394	0.0908
GOOF	1.012	1.025	1.085
$R1$ [$I > 2\sigma(I)$]	0.0650	0.0849	0.0632
$wR2$ [$I > 2\sigma(I)$]	0.1265	0.2413	0.1467
$R1$ (all data)	0.1437	0.0950	0.0960
$wR2$ (all data)	0.1589	0.2524	0.1611

Table S6 data of G-phase and O-phase under applied pressure.

G-phase			O-phase		
P (GPa)	λ (nm)	k (nm GPa^{-1})	P (GPa)	λ (nm)	k (nm GPa^{-1})
0.00	513	29.1	0.00	573	33.2
0.81	524		0.36	583	
2.06	572		0.93	601	
3.19	597		1.50	613	
3.41	618		2.02	640	
4.03	632				
4.55	648				
5.27	661				

Table S7 Optimized lattice parameters of G-phase under external stress of 0, 1, 2 and 3 GPa.

Stress/GPa	a/Å	b/Å	c/Å	α/°	β/°	γ/°	V/$Å^3$
Exp. Data	9.449	9.838	16.546	95.704	102.599	110.032	1392.04
0.0	11.055	10.655	17.540	101.311	108.419	101.589	1857.07
1.0	9.671	9.733	16.478	97.367	101.541	107.559	1419.20
2.0	9.234	9.527	16.236	96.061	100.449	109.271	1304.60
3.0	8.956	9.420	16.108	95.846	99.668	100.200	1238.42

Table S8 Optimized lattice parameters of O-phase under external stress of 0, 1, 2 and 3 GPa.

Stress/GPa	a/Å	b/Å	c/Å	α/°	β/°	γ/°	V/Å^3
Exp. Data	9.358	32.856	9.364	90.000	106.420	90.000	2761.66
0.0	10.405	32.991	11.159	90.000	102.353	90.000	3849.73
1.0	9.607	32.685	9.340	90.000	105.942	90.000	2819.82
2.0	9.301	32.582	8.968	90.000	107.310	90.000	2594.84
3.0	9.179	32.407	8.445	90.000	104.449	90.000	2432.46

Table S9 Roll angles of G-phase under external stress of 0, 1, 2 and 3 GPa.

Stress/GPa	θ_1	θ_2	θ_3	θ_4
Exp. Data	35.1	62.3	74.3	32.5
0.0	34.4	48.1	49.8	34.9
1.0	31.1	53.3	64.3	33.4
2.0	28.2	51.0	67.1	29.0
3.0	26.9	49.5	68.9	27.9

Table S10 Roll angles of O-phase under external stress of 0, 1, 2 and 3 GPa.

Stress/GPa	θ_1	θ_2	θ_3	θ_4
Exp. Data	21.2	51.5	58.6	19.8
0.0	34.4	48.1	49.8	34.9
1.0	25.6	42.5	52.8	23.3
2.0	24.2	41.8	53.8	21.6
3.0	9.2	39.6	56.7	4.4