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

Substituent Effect on the Intermolecular Interactions and Emission Behaviors in Pyrene-Based Mechanochromic Luminogens

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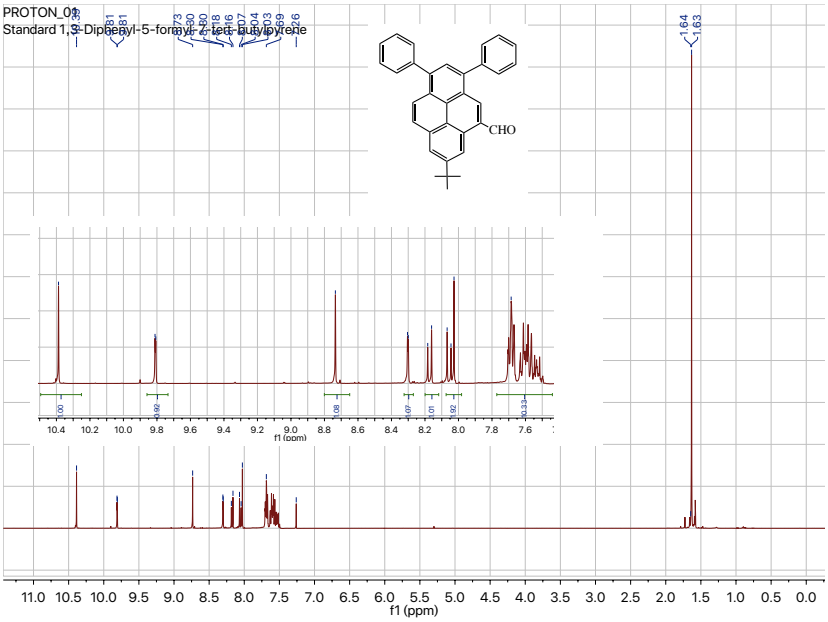


Figure S1 ^{1}H-NMR spectrum of **2** (400 MHz, 293 K, $CDCl_3$).

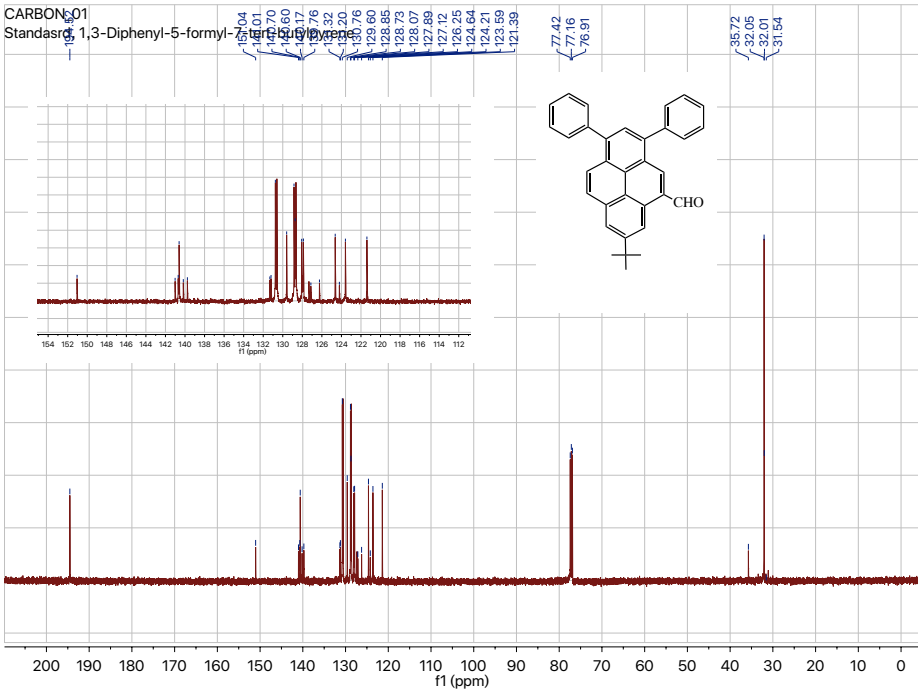


Figure S2 ^{13}C-NMR spectrum of **2** (100 MHz, 293 K, $CDCl_3$).

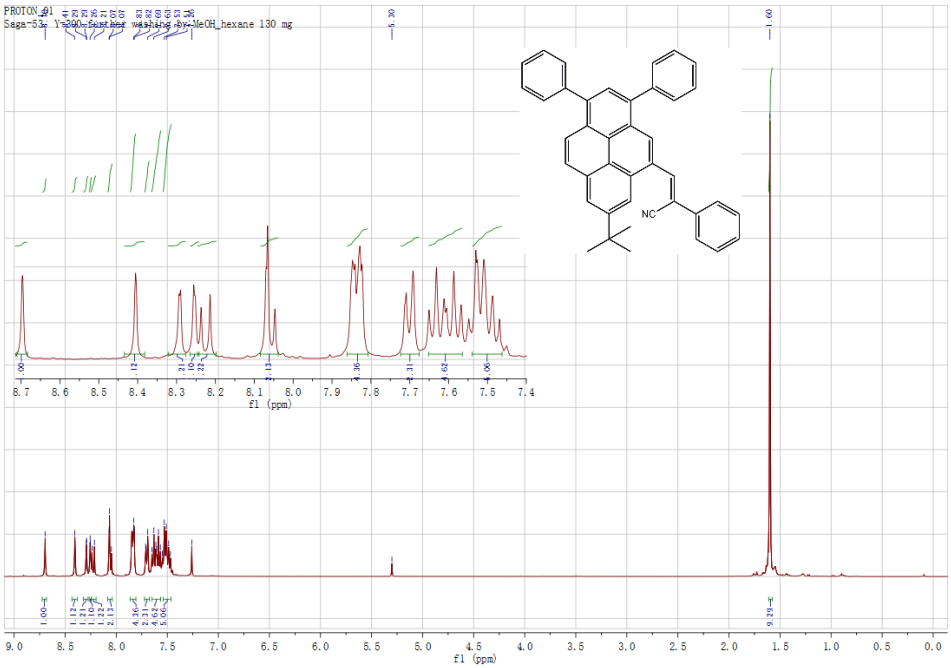


Figure S3 ^{1}H-NMR spectrum of **3a** (400 MHz, 293 K, $CDCl_3$).

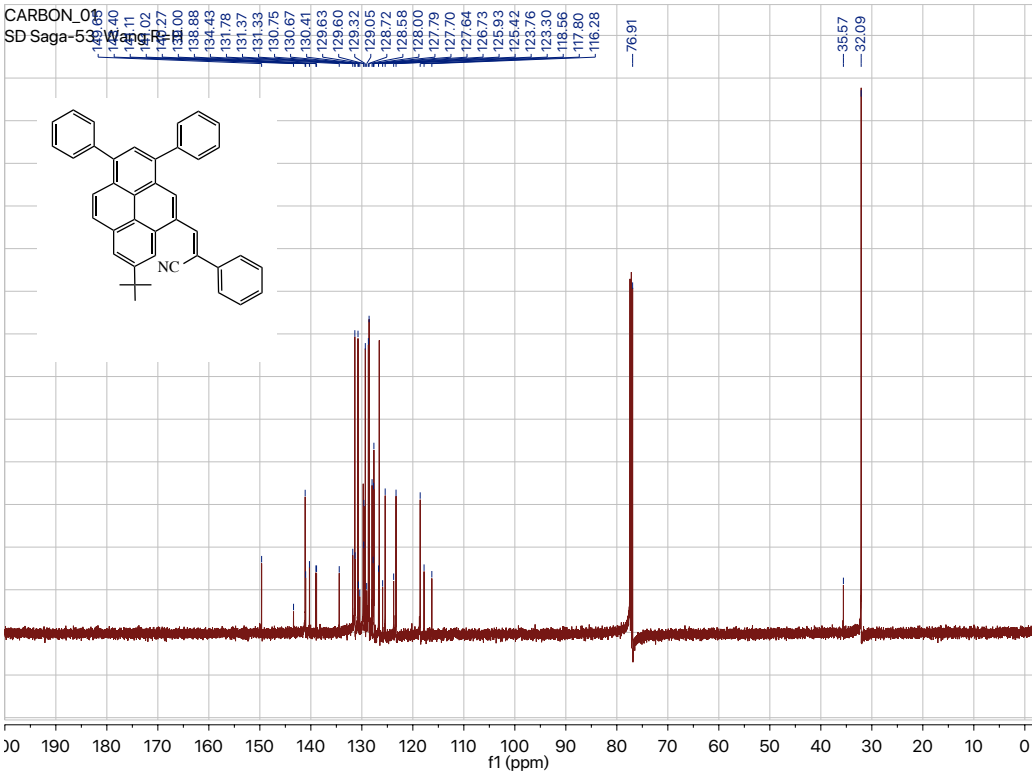


Figure S4 ^{13}C-NMR spectrum of **3a** (100 MHz, 293 K, $CDCl_3$).

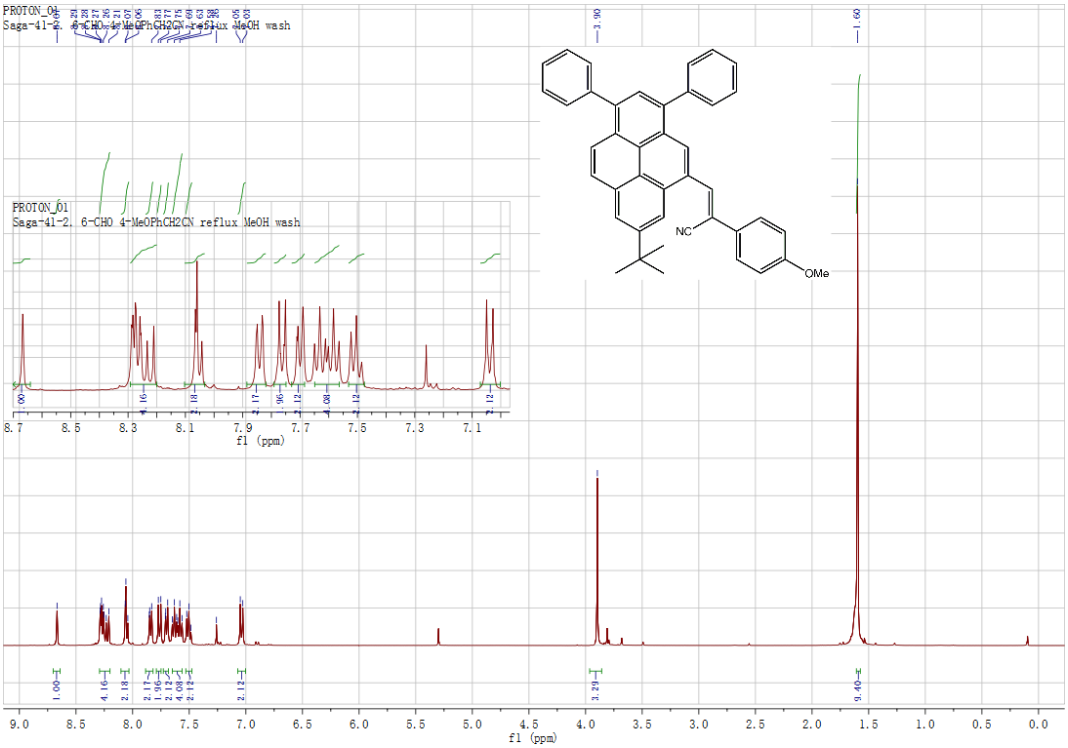


Figure S5 ^{1}H-NMR spectrum of **3b** (400 MHz, 293 K, $CDCl_3$).

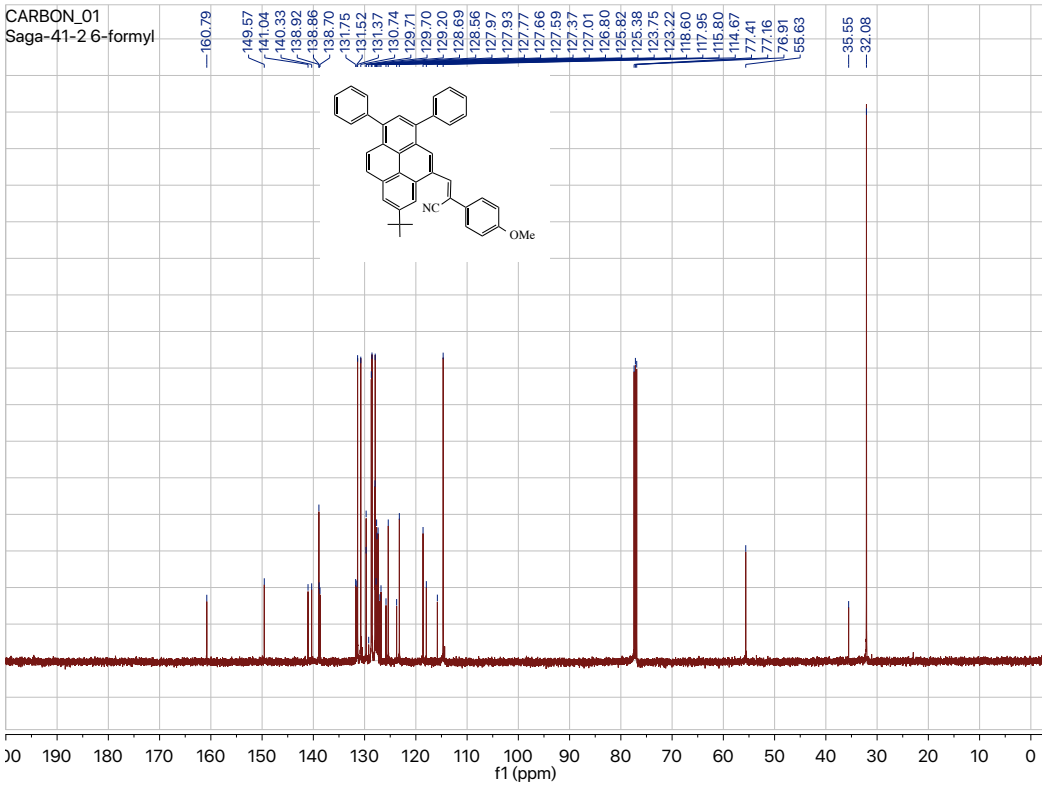


Figure S6 ^{13}C-NMR spectrum of **3b** (100 MHz, 293 K, $CDCl_3$).

Table S1 Crystal data and structure refinement of **3a** and **3b**. [a, b]

Compounds	**3a**	**3b**
Empirical formula	$C_{41}H_{31}N$	$C_{42}H_{33}NO$
Formula weight	537.67	567.69
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/c$
a[Å]	14.3989(2)	14.07592(14)
b[Å]	11.5155(2)	21.5569(3)
c[Å]	17.4968(2)	9.90225(9)
α[°]	90.00	90.00
β[°]	101.1600(10)	94.3574(9)
γ[°]	90.00	90.00
Volume[Å^3]	2846.29(7)	2995.99(6)
Z	4	4
μ	0.545 mm^{-1}	0.571 mm^{-1}
F(000)	1136	1200
Crystal size[mm^3]	0.145 × 0.069 × 0.049	0.247 × 0.068 × 0.067
Dcalcd[Mg/m^3]	1.255	1.259
Temperature [K]	100(2)	100(2)
Measured reflns	36310	38174
Unique reflns	6275	6275
Observed reflns	5968	5339
Parameters	382	402
R(int)	0.0498	0.0571
$R[I> 2\sigma(I)]$[a]	0.0421	0.0436
$wR2$[all data][b]	0.1054	0.11228
GOF on F^2	1.029	1.056

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$) [b]w$R_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; w $=1/[\sigma^2(F_o^2) + (0.095P)^2]$; $P = [\max(F_o^2, 0) + 2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

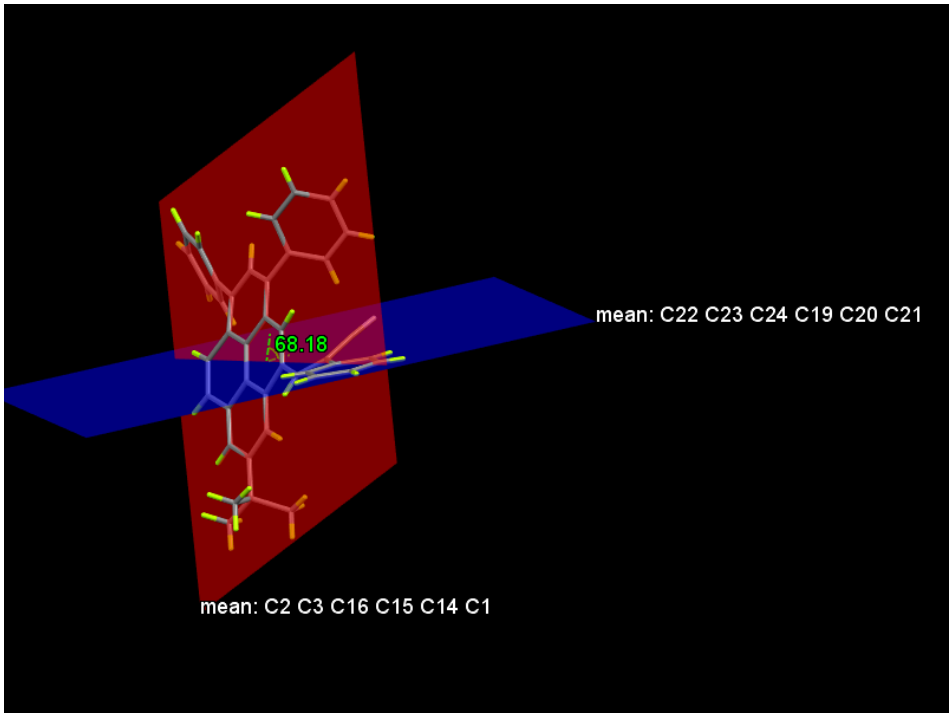


Figure S7 The dihedral angle between the pyrene core and the C_6 aromatic moiety of compound **3a**.

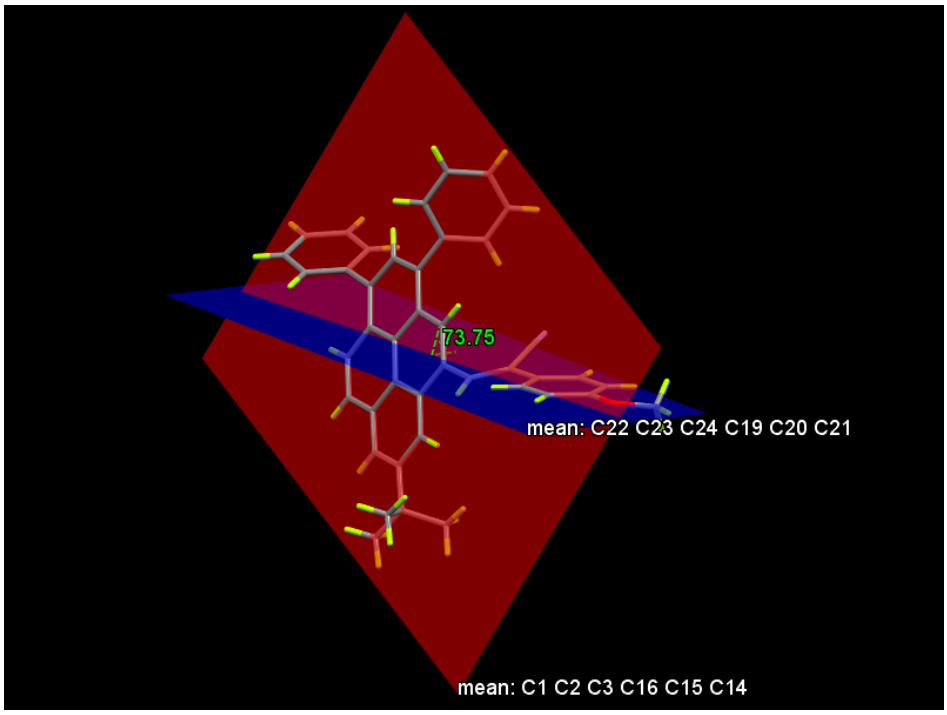


Figure S8 The dihedral angle between the pyrene core and the C_6 aromatic moiety with methoxy group of compound **3b**.

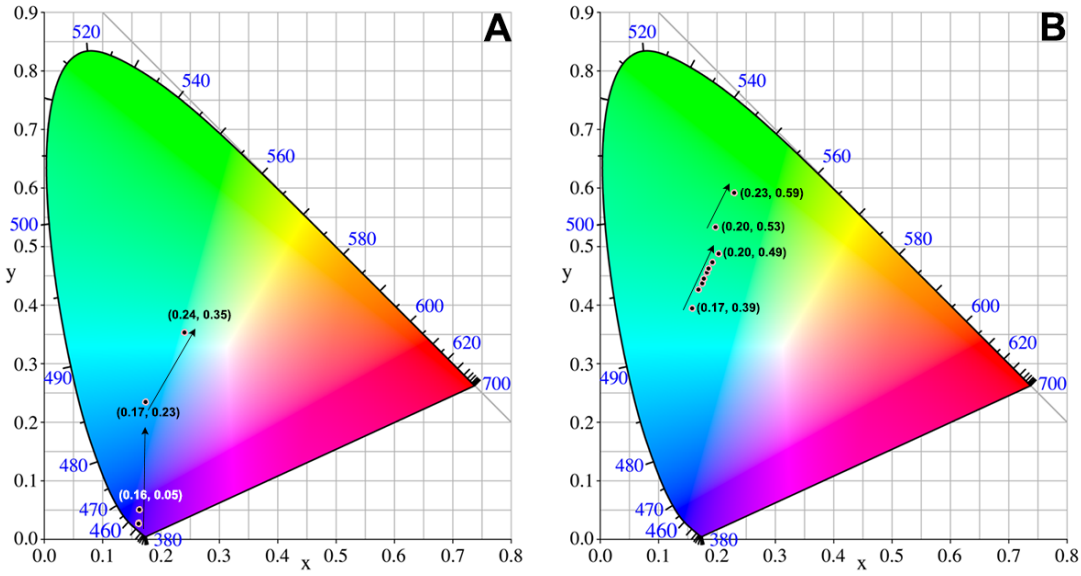


Figure S9 CIE 1931 chromaticity diagram and the color coordinates for **3a** (A), and **3b** (B) in mixture solution of H_2O/THF.

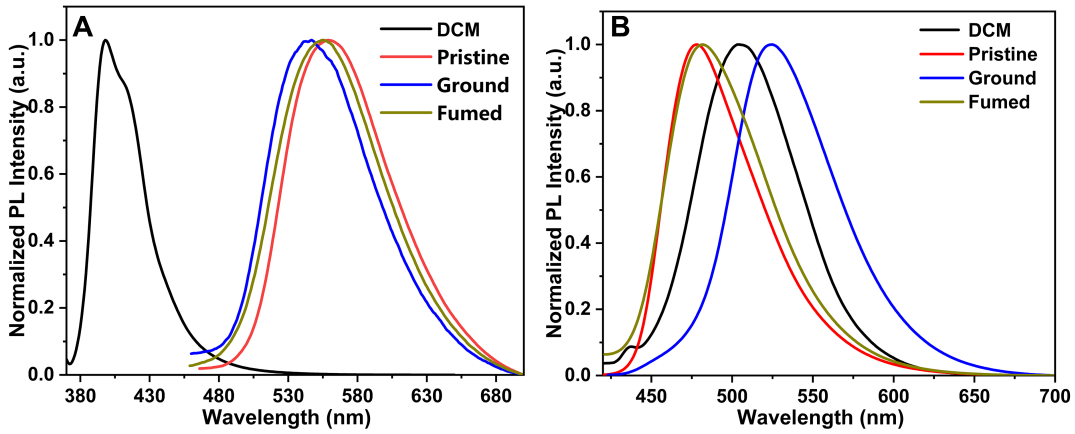
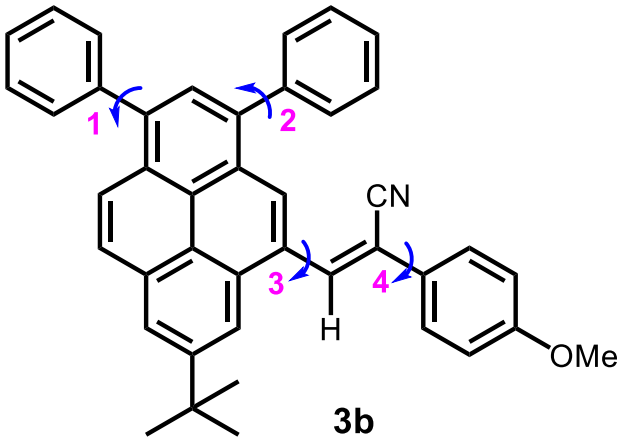


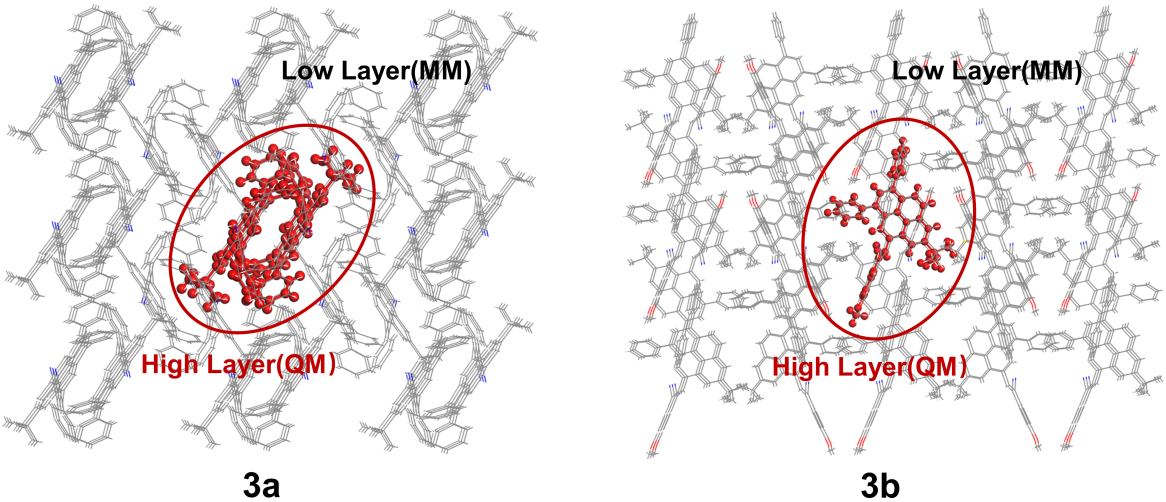
Figure S10 The emission spectra of **3a** (A) **3b** (B) in different states.

Table S2 Selected dihedral angles (in deg.) for **3b** in the pristine and ground states. S_0/S_1 and Δ represent the geometric parameters extracted from the optimized S_0/S_1 states and the modifications between two states, respectively.



3b

Locations	Pristine			Ground		
	S_0	S_1	Δ	S_0	S_1	Δ
1	−54.34	−52.25	2.09	−52.03	−46.71	5.32
2	−56.16	−52.51	3.65	−48.49	−42.14	6.35
3	47.35	39.23	8.12	39.98	23.90	16.08
4	20.70	22.93	2.23	26.44	19.77	6.67



3a **3b**

Figure S11 Setup of the ONIOM models for **3a-b**.

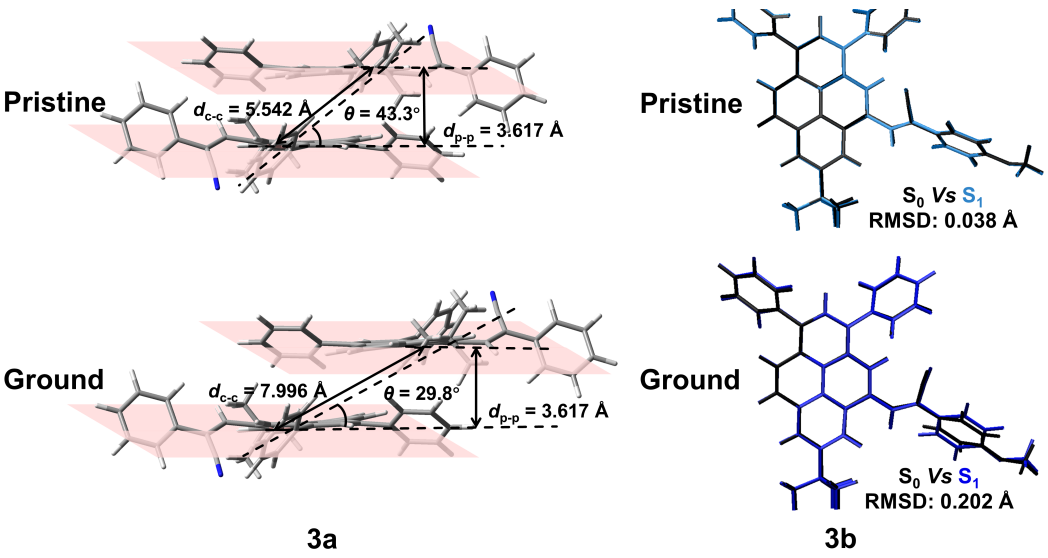


Figure S12 The molecular packing motif for the pristine and ground for **3a-b**.