Supporting Information

Solid-state photochromic properties of indole thiosemicarbazones with aggregation-induced emission

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1. Figure section

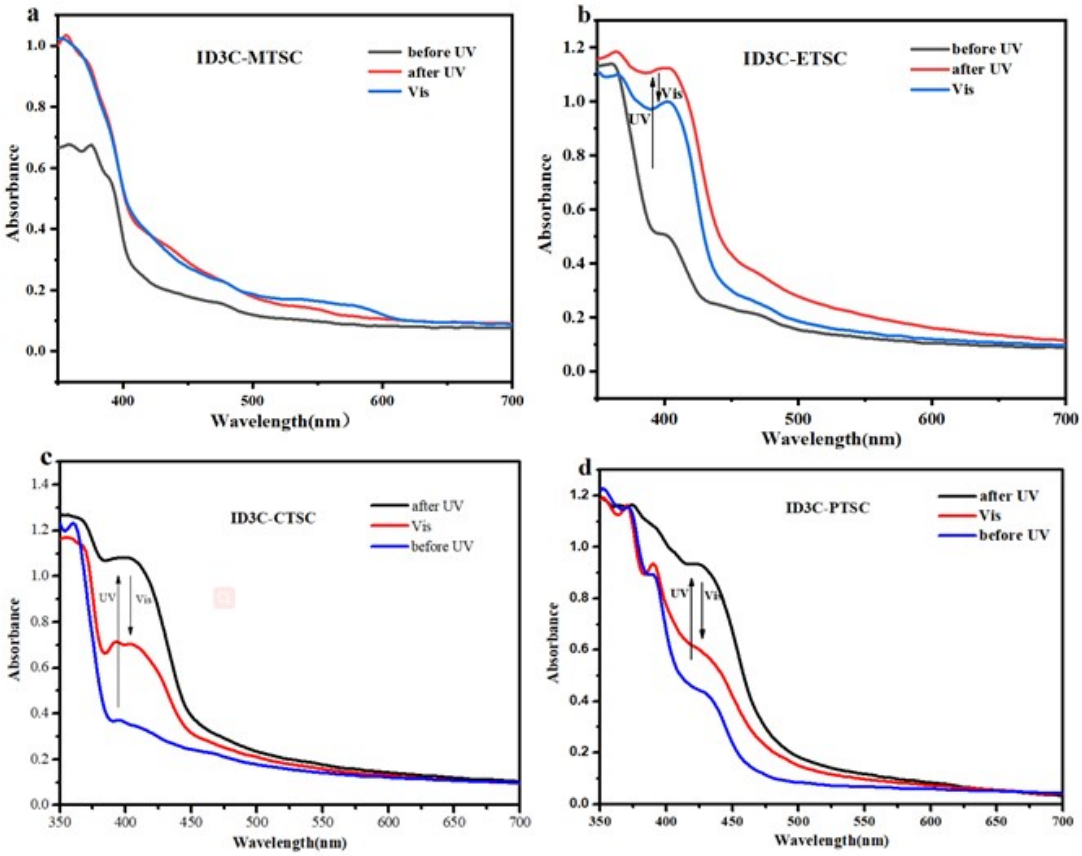

Figure S1 UV−Vis spectra of (a) ID3C-MTSC, (b) ID3C-ETSC, (c) ID3C-CTSC, and (d) ID3C-PTSC before, after 365nm irradiation, and after visible irradiation.

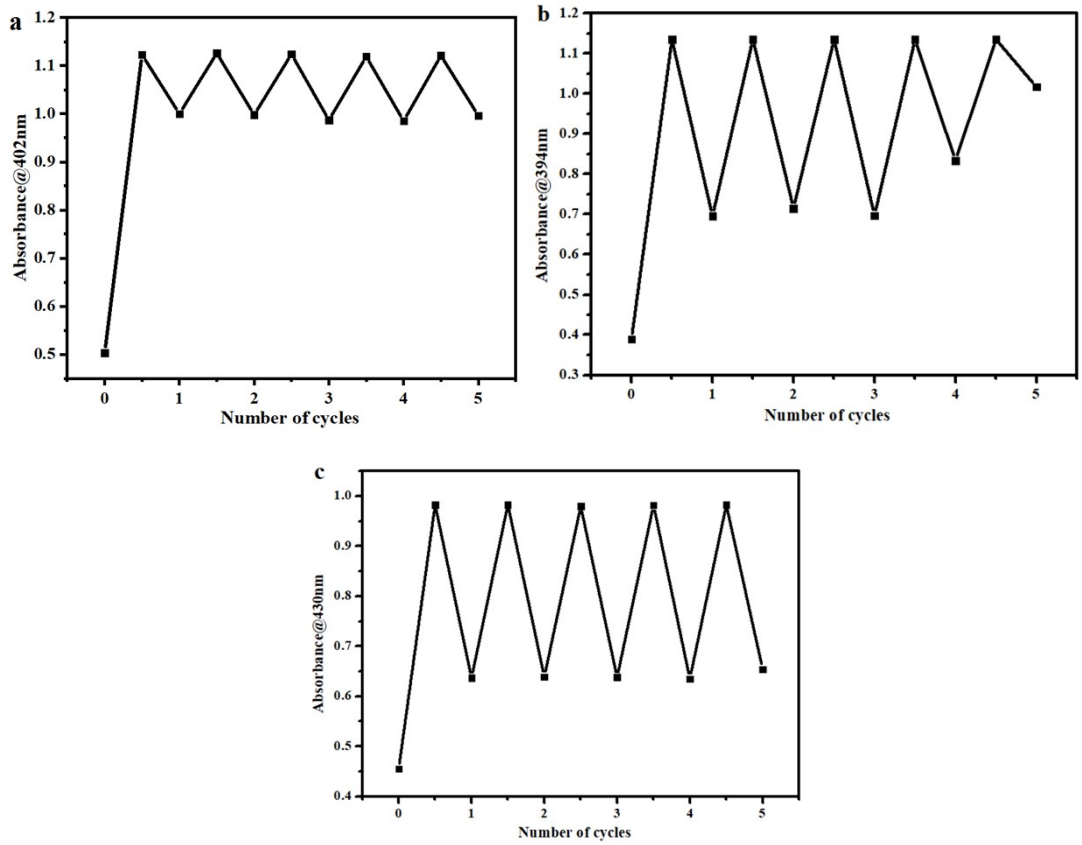

Figure S2 Photochromic cycles of (a) ID3C-ETSC, (b) ID3C-CTSC, and (c) ID3C-PTSC under irradiation of 365 nm light and visible light.

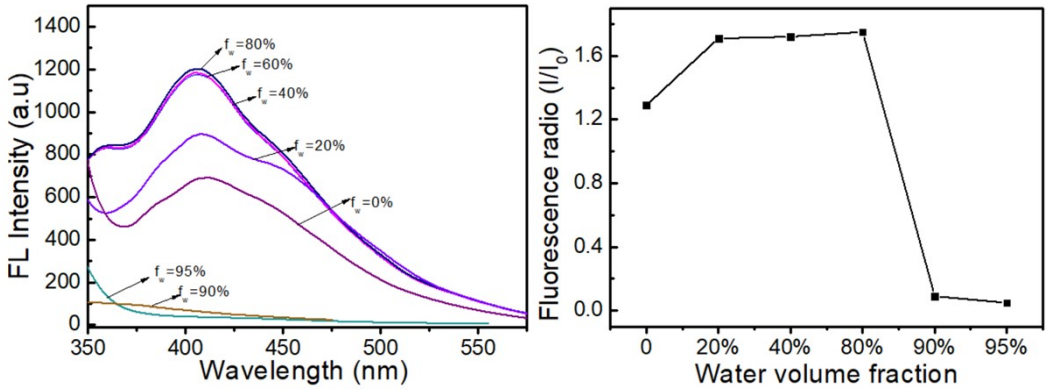

Figure S3 Fluorescence emission (left) and fluorescence radio (I/I0) (right) of THF with increasing water.

2. **Table section**

Table S1. Torsion angel of ID3C-PTSC in THF and water

	In THF		In water	
	S_0	S_1	S_0	S_1
N2-N3-C10-N4	0.05053	-0.01162	0.02522	-0.00141
C9-N2-N3-C10	179.94499	179.90334	179.96169	179.98796

In order to confirm that the enhanced fluorescence emission of ID3C-PTSC was related to RIR, the first singlet state of ID3C-PTSC in THF and water was optimized with the B3LYP functional and 6−31G (d) basis sets. The torsion angel of N2-N3-C10-N4 and C9-N2-N3-C10 was displayed in Table S1. The torsion angel of N2-N3-C10-N4 and C9-N2-N3-C10 was changed 0.02663 and 0.02627 from ground state (S_0) to the first singlet state (S_1) in water, respectively, which were less than in THF (0.06215 for N2-N3-C10-N4, 0.04165 for C9-N2-N3-C10). The result indicate that the water can restrict the intramolecular rotation and further confirmed that the enhanced fluorescence emission of ID3C-PTSC was related to RIR

Table S2. Crystal data and structure refinement for ID3C-ETSC

Compound	**ID3C-ETSC**
Empirical formula	$C_{12}H_{14}N_4S$
Formula weight	246.33
Temperature/K	193.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.106(4)
b/Å	4.9258(12)
c/Å	16.520(4)
α/°	90
β/°	99.557(12)
γ/°	90
Volume/Å3	1212.2
Z, Calculated density	4, 1.350g/cm3

Compound	**ID3C-ETSC**
Empirical formula	$C_{12}H_{14}N_4S$
μ/mm-1	1.461
F(000)	520.0
Crystal size/mm3	0.12 × 0.1 × 0.1
Radiation	Ga Kα (λ =1.34139)
Theta range for data collection/°	9.446 to 122.934
Index ranges	-18 ≤ h ≤ 19, -6 ≤ k ≤ 5, -21≤ l ≤ 17
Reflections collected	10113
Independent reflections	2776 [Rint = 0.0547, Rsigma = 0.0470]
Data/restraints/parameters	2776/0/155
Goodness-of-fit on F2	1.134
Final R indexes [I⩾2σ (I)]	R1 = 0.0452, wR2 = 01216
Final R indexes [all data]	R1 = 0.0600, wR2 = 0.1321
Largest diff. peak/hole / e Å-3	0.27/-0.39

Table S3. Bond lengths for ID3C-ETSC

Bonds	**Length/Å**	**Bonds**	**Length/Å**
S1-C10	1.6896(19)	C1-C6	1.407(3)
N1-C1	1.379(3)	C2-C3	1.377(4)
N1-C8	1.353(3)	C3-C4	1.392(4)
N2-N3	1.377(2)	C4-C5	1.375(3)
N2-C9	1.287(2)	C5-C6	1.397(3)
N3-C10	1.343(2)	C6-C7	1.441(3)
N4-C10	1.330(2)	C7-C8	1.376(3)
N4-C11	1.447(2)	C7-C9	1.428(3)
C1-C2	1.390(3)	C11-C12	1.503(3)

Table S4. Bond angles for ID3C-ETSC

Bonds	**Angle(˚)**	**Bonds**	**Angle(˚)**
C8-N1-C1	109.15(16)	C5-C6-C1	118.75(19)

C9-N2-N3	116.01(16)	C5-C6-C7	134.93(18)
C10-N3-N2	119.39(15)	C8-C7-C6	106.43(18)
N1-C1-C2	129.6(2)	C8-C7-C9	124.58(19)
N1-C1-C6	107.93(18)	C9-C7-C6	128.92(17)
C2-C1-C6	122.4(2)	N1-C8-C7	110.17(19)
C3-C2-C1	117.5(3)	N2-C9-C7	121.26(318)
C2-C3-C4	121.9(2)	N3-C10-S1	120.58(14)
C5-C4-C3	120.9(2)	N4-C10-S1	123.06(14)
C4-C5-C6	119.1(2)	N4-C10-N3	116.34(16)
C1-C6-C7	106.32(18)	N4-C11-C12	110.04(19)

Table S5. Hydrogen Bonds for ID3C-ETSC

D-H…A	**d(H…A)**	**d(D-H)**	**d(D…A)**	**∠(DHA)**
N1-H1…S1	0.88	2.5693(4)	3.4442(19)	172.851(16)
N3-H3…S1	0.88	2.6726(6)	3.3810(17)	138.474(14)

Table S6 HOMOs and LUMOs of the four compounds calculated with B3LYP/6-311+G(d) level

compound	Electronc transition	Energy (eV)	Oscillator strengths	Composition	Transition type	Egap
ID3C-MTSC	$S_0 \rightarrow S_2$	3.82eV/324.53nm	0.4291	H→L	π→π*	4.18
ID3C-ETSC	$S_0 \rightarrow S_2$	3.83eV/323.03nm	0.4654	H-1→L	π→π*	4.17
ID3C-CTSC	$S_0 \rightarrow S_2$	3.81eV/325.43nm	0.4436	H-1→L	π→π*	4.16
ID3C-PTSC	$S_0 \rightarrow S_2$	3.70eV/334.46nm	0.8249	H→L	π→π*	4.02