Electronic Supplementary Information

Pure White Light Emission from Organic Molecules Using Solvent Induced Selective Self-Assembly

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Materials and methods:

Materials: 9-Anthracecarboxaldehyde was purchased from Sigma-Aldrich, 9anthracecarboxylic acid and rhodamin B were purchased from SpectrochemPvt. Ltd. Acetonitrile, water, methanol HPLC grade were purchased from SpectrochemPvt. Ltd. Acetonitrile d_3 was purchased from Cambridge Isotope Laboratories and water d_2 was purchased from Sigma-Aldrich.

Gel preparation: 1.6 g of agar-agar was dissolved in the 100 mL of distilled water and heated to dissolve. 2.250 mL hot agar-agar solution was mixed with 0.250 mL acetonitrile solution of desired emitters.

UV-Visible absorption experiments: Absorption spectra were recorded in Jasco V-660 UVvisible spectrophotometer. Sample solutions are taken in 10 mm, 5mm or 2 mm quartzcell. In order to take absorption spectra of the aggregates, solution are sonicated and stabilized for 6 hour.

Fluorescence experiments: Emission Spectra were recorded in Horiba Jovinyvon Fluoromax-4 spectrofluorometer. A four-face transparent quartzcuvette with 10 mm path length was used. The emissions from thesample were monitored at a 90° angle with respect to the excitation light source with excitation and emission slit of 2 nm. Variable temperature emission spectra was recorded while cooling the solutions from 90 °C to 0 °C with 5 °C interval after 5 minute stabilisation in same spectrometer equipped with Peltier thermostat. Fluorescence spectra of the hydrogel were taken by putting the hydrogel into solid state holder. Quantum yield of emission was determined using quinine sulphate as a standard ($\phi = 0.57$ in 0.1M H₂SO₄; excitation wavelength = 360 nm).¹

NMR experiments:Nuclear Magnetic Resonance (NMR) spectra were recorded in Bruker 500 MHz instrument. 0.5 mL of solution was taken in a 5 mm diameter NMR tube. Prior to perform NMR experiment solutions were stabilized for 6 hour.

Time correlated single photon counting experiments: Time-resolved luminescence decay experiments were recorded on a Horiba JobinYvonFluoroCube instrument in a time-correlated single-photon-counting (TCSPC) arrangement. A 370 nm nano-LED with a pulse repetition rate of 1 MHz was used as the light source. The instrument response function (IRF) was collected by using a scatterer (Ludox AS40 colloidal silica, Sigma-Aldrich). For the 370nm LED light source, the instrumental full width at half-maximum including detector response was ~ 1.2 ns.

Scanning Electron Microscopy: Scanning electron microscopy (SEM) images are captured with Hitachi S-4800 FE SEM instrument. Sample solution was drop casted over Indium Tin oxide (ITO) coated Glass and gold coating was done prior to take images.



Figure S1: UV-visible absorption spectra ofAnC60 μ M for variable water concentration in acetonitrile-water; black solid line (ϕ_w 00), red solid line (ϕ_w 0.20), blue solid line (ϕ_w 0.40), green solid line (ϕ_w 0.50), cyan solid line (ϕ_w 0.60), cyan dotted line (ϕ_w 0.70), green dotted line (ϕ_w 0.80), blue dotted line (ϕ_w 0.90), red dotted line (ϕ_w 0.95) and black dotted line (ϕ_w 0.96)



Figure S2: UV-visible absorption spectra of AnC $60\mu M$ for variable water concentration in methanol-water.



Figure S3: UV-visible absorption spectra of AnC 60μ M for variable water concentration in ethanol-water.



Figure S4: UV-visible absorption spectra of AnC 60μ M for variable water concentration in propanol-water.



Figure S5: Variable concentration NMR spectra (partial) of AnC in CD₃CN-D₂O (9:1).



Figure S6: NMR spectra (partial) of AnC (12 mM) in CD_3CN-D_2O mixture with variable D_2O concentrations.



Figure S7: SEM image of the AnC in acetonitrile-water ϕ_w 0.96 a. 60 μ M, b. 120 μ M



Figure S8: UV-visible absorption spectra of AnA $60\mu M$ for variable water concentration in acetonitrile-water.



Figure S9: Variable concentration UV-visible absorption spectra for AnA in acetonitrile-water mixture at ϕ_w 0.96.



Figure S10: Plot of molar absorption coefficient of 380nm and 380 nmvs concentration in acetonitrile-water mixture at ϕ_w 0.96.



Figure S11: Emission spectra of AnA $60\mu M$ for variable water concentration in acetonitrile-water upon350 nm excitation.



Figure S12: Variable concentration emission spectra for AnA in acetonitrile-water mixture at $\phi_w 0.96$ upon 370 nm excitation.



Figure S13: NMR spectra (partial) of AnA (12 mM) in CD_3CN-D_2O mixture with variable D_2O concentrations



Figure S14: Emission spectra for AnC 60μ M variable water concentration in Acetonitrilewater upon 405 nm excitation.



Figure S15: plot of 405 nm absorbance and 515 nm emission vs water content for AnC $60\mu M$ in Acetonitrile-water.



Figure S16: Emission spectra for AnC 60μ M variable water concentration in methanol-water upon 405 nm excitation.



Figure S17: Emission spectra for AnC 60μ M variable water concentration in ethanol-water upon 405 nm excitation.



Figure S18: Emission spectra for AnC 60μ M variable water concentration in propanol-water upon 405 nm excitation.

Table S1: Quantum yield of AnC and AnA

Solvent system	Quantum yield of AnC	Quantum yield of AnA
Acetonitrile	-	0.24±0.003
Acetonitrile-water(ϕ_w 0.90)	0.04±0.001	0.09±0.001



Figure S19: Time resolved emission decay for AnC 60 μ M in acetonitrile-water at ϕ_w 0.96 at variable emission wavelength.



Figure S20: variable concentration time resolved emission decay for AnC in acetonitrilewater at $\varphi_w 0.96.$



Figure S21: variable water content time resolved emission decay for AnC 60 μ M.



Figure S22: Variable temperature emission spectra in acetonitrile- water for AnC 60 μ M at ϕ_w 0.90



Figure S23:Variable temperature emission spectra in ethanol- water for AnC 60 μ M at ϕ_w 0.90.



Figure S24: Variable temperature emission spectra in propanol- water for AnC 60 μ M at ϕ_w 0.90.



Figure S25: Plot of 515 nm emission intensity vs temperature in acetonitrile-water, propanol-water and ethanol-water mixture at $\phi_w 0.90$.



Figure S26: Plot of emission intensity from AnC at 515 nm vs concentration in acetonitrilewater at $\phi_w 0.96$.



Figure S27: Variable concentration emission spectra of AnA in mixture with AnC 60 μ M in acetonitrile-water at ϕ_w 0.90.



Figure S28: variable excitation wavelength emission spectra for AnC 60 μ M and AnA 36 μ M mixture in acetonitrile-water at ϕ_w 0.90.



Figure S29: Time resolved emission decay of 30 μ M AnA in acetonitrile.



Figure S30: Time resolved emission decay of 30 μ M AnA in acetonitrile-water ϕ_w 0.90.



Figure S31: Time resolved emission decay of 30 μ M AnA in mixture with AnC 60 μ M in acetonitrile-water ϕ_w 0.90.



Figure S32: Time resolved emission decay of 16 μ M AnA in mixture with AnC 60 μ M and RhB 10 μ M in acetonitrile-water ϕ_w 0.90.



Figure S33: Time resolved emission decays of AnC 60 μM in mixture with 36 μM AnA in acetonitrilewater $\varphi_w 0.90.$



Figure S34: Time resolved emission decay of AnC 60 μM in mixture with10 μM RhB in acetonitrilewater $\phi_w 0.90.$



Figure S35: Time resolved emission decay of AnC 60 μ M in mixture with 16 μ M AnA and RhB 10 μ M in acetonitrile-water ϕ_w 0.90.



Figure S36: Time resolved emissiondecay of RhB 10 μ M in acetonitrile-water ϕ_w 0.90.



Figure S37: Time resolved emissions decay of RhB 10 μ M in mixture with AnA 60 μ M in acetonitrile-water at ϕ_w 0.90.



Figure S38: Time resolved emissions decay of RhB 10 μ M in mixture with AnC 60 μ M and AnA 16 μ M in acetonitrile-water at ϕ_w 0.90.

Table S2: Excited-State Decay Parameters of AnC obtained from TCSPC measurement for AnC 60 μ Min acetonitrile-water at ϕ_w 0.90

Emission wavelength (nm)	Lifetime (ns)	Chi sq.
475	1.64	1.24
500	1.59	1.10
525	1.56	1.18
550	1.57	1.12
575	1.58	1.11
600	1.56	1.08
625	1.56	1.12
650	1.55	1.16
700	1.57	1.18

Table S3: Excited-State Decay Parameters of AnC obtained from TCSPC measurement for various concentration of AnC in acetonitrile-water at $\phi_w 0.90$

concentration	Life time ns	Chi sq.
30	1.59	1.16
60	1.56	1.02
90	1.61	1.08
120	1.60	1.04

Table S4: Excited-State Decay Parameters of 60 μ M AnC obtained from TCSPC measurement for various water content in acetonitrile-water mixture at ϕ_w 0.90.

Fraction of water	Life time ns	chisq
0.6	0.64	1.17
0.7	0.95	1.21
0.8	1.34	1.25
0.9	1.62	1.16
0.96	1.56	1.02

Table S5: Excited-State Decay Parameters obtained from TCSPC measurement.

material	Solvent	wavelength	Lifetime (ns)	chisq	remarks
	system				
AnC	Methanol-	525 nm	1.67	1.05	excimer
	water				
AnC	Ethanol-water	525 nm	1.59	1.29	excimer
AnA	Acetonitrile-	435 nm	1.25	1.12	monomer
	water				
RhB	Acetonitrile	650 nm	1.61	1.18	monomer
	water				
AnA	acetonitrile	480 nm	5.44	1.01	excimer



Figure S39: Variable temperature emission spectra of AnA 36 μ M andAnC60 μ M mixture in acetonitrile-water mixture at ϕ_w 0.9.



FigureS40: Variable temperature emission spectra of AnA 14 μ M, AnC 60 μ M andRhB10 μ M mixture in acetonitrile-water mixture at ϕ_w 0.9.



Figure S41: Variable temperature emission spectra of AnA 17 μ M, AnC 60 μ M and RhB 10 μ M mixture in acetonitrile-water mixture at ϕ_w 0.9.



Figure S42: Variable temperature emission spectra of AnA 20 μ M, AnC 60 μ M and RhB 10 μ M mixture in acetonitrile-water mixture at ϕ_w 0.9.



Figure S43: Various concentration scattering removed emission spectra of various concentrations of AnA, AnC 60 μ M and RhB 10 μ M in agar-agar hydrogel (acetonitrile-water mixture at ϕ_w 0.9).

Table S6: CIE coordinates obtained from emission spectra of various concentration AnA and AnC 60 μ M in acetonitrile-water mixture at ϕ_w 0.9.

AnAμM	CIE coordinates
0	0.28, 0.52
18	0.23, 0.35
24	0.23, 0.33
30	0.22, 0.31
36	0.22, 0.29
42	0.21, 0.28
48	0.21, 0.26
54	0.20, 0.25
60	0.20. 0.24
72	0.20, 0.23

Table S7: CIE coordinates obtained from emission spectra of various concentration AnA, AnC 60 μ M and RhB 10 μ M in acetonitrile-water mixture at ϕ_w 0.9.

ΑηΑμΜ	CIE coordinates
0	0.40,0.46
5	0.37, 0.40
10	0.35, 0.37
15	0.34, 0.35
16	0.33, 0.33
20	0.32, 0.32
25	0.31, 0.31
30	0.30, 0.28

Table S8: CIE coordinates obtained from emission spectra of variable temperature experiments in a mixture of AnA 36 μ M and AnC 60 μ M in acetonitrile-water mixture at ϕ_w 0.9.

Temperature deg C	CIE coordinates
90	0.20, 0.24
85	0.20, 0.25
80	0.20, 0.26
75	0.21, 0.28
70	0.21, 0.29
65	0.21, 0.31
60	0.22, 0.32
55	0.22, 0.34
50	0.23, 0.36
45	0.23, 0.37
40	0.23, 0.39
35	0.24, 0.40
30	0.24, 0.42
25	0.25, 0.43
20	0.25, 0.43
15	0.24, 0.39
10	0.23, 0.35
5	0.22, 0.32
0	0.22, 0.30

Table S9: CIE coordinates obtained from emission spectra of variable temperature experiments in a mixture of AnA, AnC 60 μ M and RhB 10 μ M in acetonitrile-water mixture at ϕ_w 0.9.

Temperature deg C	CIE coordinates for	CIE coordinates for	CIE coordinates for
	AnA 14 μM, AnC	AnA 17 μM, AnC	AnA 20 μM, AnC
	60μM, RhB 10 μM	60μM, RhB 10 μM	60μM, RhB 10 μM
90	0.26, 0.26	0.26, 0.25	0.23, 0.20
85	0.26, 0.27	0.26, 0.26	0.24, 0.21
80	0.27, 0.27	0.27, 0.27	0.24, 0.22
75	0.27, 0.28	0.27, 0.28	0.24, 0.23
70	0.28, 0.29	0.28, 0.29	0.25, 0.24

65	0.28, 0.30	0.29, 0.29	0.26, 0.25
60	0.29, 0.31	0.29, 0.30	0.26, 0.26
55	0.30, 0.32	0.30, 0.31	0.27, 0.27
50	0.31, 0.33	0.31, 0.32	0.28, 0.28
45	0.31, 0.34	0.32, 0.33	0.28, 0.29
40	0.32, 0.35	0.32, 0.34	0.29, 0.30
35	0.33, 0.36	0.33, 0.35	0.30, 0.31
30	0.33, 0.37	0.34, 0.36	0.31, 0.32
25	0.34, 0.37	0.34, 0.37	0.32, 0.33
20	0.35, 0.36	0.36, 0.37	0.33, 0.33
15	0.36, 0.35	0.38, 0.37	0.33, 0.32
10	0.37, 0.31	0.40, 0.36	0.33, 0.30
5	0.38, 0.31	0.40, 0.36	0.34, 0.28
0	0.39, 0.31	0.40, 0.35	0.34, 0.27

Table S10: CIE coordinates obtained from emission spectra of various concentration AnA and AnC 60 μ M in agar-agar gel (acetonitrile-water mixture at ϕ_w 0.9).

AnAμM	CIE coordinates
7	0.21, 0.31
14	0.20, 0.24
21	0.19, 0.22
28	0.19, 0.18
35	0.18, 0.15
42	0.17, 0.13
49	0.17, 0.12
56	0.17, 0.11

Table S11: CIE coordinates obtained from emission spectra of various concentration AnA, AnC 60 μ M and RhB 10 μ M in agar-agar gel (acetonitrile-water mixture at ϕ_w 0.9).

variable	Cie gel
7	0.34, 0.36
10	0.33, 0.33
14	0.30, 0.29
17	0.28, 0.26
21	0.28, 0.25
24	0.27, 0.24
28	0.26, 0.22

Nucleation elongation:

Supramolecular polymerisation can takes place either by isodesmic or cooperative (nucleation elongation) pathway. During isodesmic polymerisation, each monomer addition

takes place with same equilibrium constant, where as in cooperative polymerisation two equilibrium exist one for nucleation and another for elongation.

Isodesmic model:

$$A \xrightarrow{K_2} A_1 \xrightarrow{K_3} A_2 \xrightarrow{K_4} A_3 \longrightarrow A_i$$

 $K_2 = K_3 = K_4 = K_i = K_i$

$$\alpha_{agg} = 1 - \alpha_{mon} = 1 - \frac{c_{mon}}{c_T} = 1 - \frac{2Kc_T + 1 - \sqrt{4Kc_T + 1}}{(2Kc_T)^2}$$

Cooperative model:

$$A \xrightarrow{K_2} A_1 \xrightarrow{K_3} A_2 \xrightarrow{K_4} A_3 \longrightarrow A_i$$

 $K_2 \neq K_3 = K_4 = = K_i = K$

$$\alpha_{agg} = 1 - \alpha_{mon} = 1 - \frac{c_{mon}}{c_T} = 1 - \frac{2Kc_T + 1 - \sqrt{4Kc_T + 1}}{(2Kc_T)^2}$$

 $\sigma = \frac{K_2}{K}$ Where,

$$\alpha_{agg} = 1 - \alpha_{agg} = 1 - \frac{Kc_{mon}}{Kc_T}$$

 K_2 = equilibrium constant for nucleation.

K= equilibrium constant for elongation.

Reference

1. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Plenum Press, New York, 1999.