Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2016

Electronic Supporting information

A Sensitive AIEE Probe for Amphiphilic Compounds

Veerabhadraiah Palakollu¹, Anuji K. Vasu¹, Vijay Thiruvenkatam²and Sriram Kanvah^{1*}

¹Department of Chemistry, Indian Institute of Technology Gandhinagar, Indian Institute of Technology Gandhinagar, Ahmedabad-382424, India. E-mail: *kanvah@gatech.edu

²Department of Biological Engineering, Indian Institute of Technology Gandhinagar, Ahmedabad 382424, e-mail <u>vijay@iitgn.ac.in</u>



Figure S1.Aggregation induced enhanced emission of Stilbene-1 as examined using dioxanewater binary mixture. (This figure was earlier published from our group in New Journal of Chemistry 38 (2014) 5736-5746 and is included for reader benefit)

Identification code	EXP2
Empirical formula	C17 H16 N2 O
Formula weight	264.32
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	Pnma
Unit cell dimensions	$a = 16.9790(10) \text{ Å}, \alpha = 90^{\circ}.$
	$b = 10.3445(9) \text{ Å}, \beta = 90^{\circ}.$
	$c = 15.9847(10) \text{ Å}, \gamma = 90^{\circ}.$
Volume	2807.5(3) Å ³
Ζ	8
Density (calculated)	1.251 Mg/m ³
Absorption coefficient	0.624 mm ⁻¹
F(000)	1120
Crystal size	0.5 x 0.2 x 0.3 mm ³
Theta range for data	3.798 to 65.970°.
collection	
Index ranges	-20<=h<=19, -12<=k<=8, -18<=l<=16
Reflections collected	6681
Independent reflections	3479 [R(int) = 0.0396]
Completeness to theta = 65.970°	99.0 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints /	3479 / 1 / 369
parameters	
Goodness-of-fit on F ²	1.130
Final R indices	R1 = 0.0566, wR2 = 0.1344
[I>2sigma(I)]	
R indices (all data)	R1 = 0.0609, WR2 = 0.1407
Absolute structure	-0.3(5)
parameter	
Extinction coefficient	0.0052(6)
Largest diff. peak and	0.270 and -0.301 e.Å ⁻³
hole	1021051
CCDC number	1031951

 Table S1: Crystal data and structure refinement for stilbene (1)

Intermolecular H-bonding interaction table:

Donor-HydrogenAcceptor	Don-Hyd [Å]	Hyd-Acc [Å]	Don-Acc [Å]	D-HA [0]
O18-H18N20A	0.82	2.04	2.836	163.4°



Figure S2. Packing diagram of stilbene (1) showing the crystallographic symmetry molecules with the glide plane and 2_1 screw axis along the symmetric equivalent positions a) 1/2+x,y,1/2-z "Glide plane perpendicular to [0, 0, 1] with glide component [1/2, 0, 0]"; b) 1/2-x,1/2+y,1/2+z "Glide plane perpendicular to [1, 0, 0] with glide component [0, 1/2, 1/2]"; c) -x,1/2+y,-z "2-fold screw axis with direction [0, 1, 0] at 0, y, 0 with screw component [0, 1/2, 0]". The dotted lines indicate intermolecular contacts.



Figure S3:Absorption spectra of stilbene (1) in SDS (1 x 10^{-3} M); Triton X-100 (5 x 10^{-5} M) and CTAB (2 x 10^{-4} M)



Figure S4: Color changes as observed using hand-held UV lamp. Clear demarcation is only seen when the micelles are formed. At above or below the CMC, the colours are uniform.



Figure S5.Fluorescence microscope images of stilbene (1) in SDS a) 1×10^{-3} M b) 15×10^{-3} M; Triton X-100 c) (5×10^{-5} M) d) 7×10^{-4} M; CTAB e) 2×10^{-4} f) 15×10^{-4} . The observed intensity changes are SDS (94 to 50), CTAB (73 to 60) and in Triton X-100 (93 to 46)].



Surfactant	Particle Size	Particle Size	RE		
	Below CMC (nm)	Above CMC (nm)	10		
SDS	354	35188.6	80		
Triton X-100	274.3	1793.5	40		
CTAB	1266.3	42558.8	20		
In Distilled Water =2234.1nm					



Figure S6. Particle size distribution of stilbene (1) in surfactants at below CMC and in water below CMC.





Figure S7. Decay profile of stilbene (1) a) in water, b) SDS, c) CTAB and d) Triton X-100

Media	$\tau_1(ns)$	τ_2 (ns)	χ^2
Water	1.40		1.075
SDS (2 mM)	0.95 (42.40%)	2.03 (57.60%)	1.013
CTAB (0.4 mM)	0.95 (58.87%)	2.40 (41.13%)	1.005
Triton X-100 (0.05 mM)	0.92 (32.15%)	1.65 (67.85%)	1.061

Table S2: Fluorescence lifetime data of stilbene in water and surfactant media