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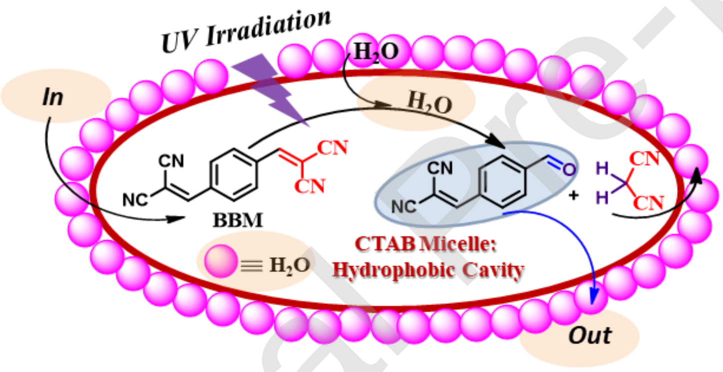
Graphical Abstract



Highlights

- Photodissociation kinetics of selective C=C bond in BBM is investigated in different micelle concentration.
- It is clear that ionic environment (in presence of KCl) does play important role on photodissociation kinetics but micelle concentration plays significant role on photodissociation kinetics.
- In micelle, hydrophobic region plays important role on enhancing rate of photodissociation.
- It can be stated that rate of photodissociation in hydrophobic environment (Specially CMC condition) is higher compared to polar protic and aprotic solvents.

Abstract: In present work, photodissociation kinetics of selective C=C bond in BBM is investigated in different micelles concentration. In polar solvents, rate of photodissociation (k) is relatively lower compared to H_2O solvent under similar condition. The rate of photodissociation (k) is enhanced with increase of aqueous CTAB concentration and found to be highly sensitive to aqueous CTAB concentration. It is clear that micelle concentration and hydrophobic region plays significant role on enhancing rate of photodissociation. Crucial role of hydrophobic region in micelle has been discussed and confirmed by experimental results.

KEYWORDS: Photodissociation; Micelle; Cetyl Trimethyl Ammonium Bromide (CTAB); Critical Micelle Concentration (CMC); Solute-Solvent Interaction.

Introduction

Photochemistry of organic molecules has been studied extensively as model system for understanding fundamental and elementary physicochemical process in solution and biological system.[1-3] The π-conjugated organic molecules have been intensively developed as an attractive platform for the design and fabrication of a wide range of nano- and microstructures for use in organic optoelectronics.[4] Photoinduced cis-trans isomerization of C=C bond is widely observed by external light stimulus and is responsible for various photochemical process like vision process, phototaxis, control of germination, and photoinduced ion pumping.[5-6] Popular trans-stilbene organic molecule shows interesting photo-induced cis-trans isomerization about a C=C bond.[7-8] The structural dynamics and solvent-induced photoisomerization of trans-stilbene have been investigated to understand fundamental mechanism of cis-trans photoisomerization.[9-11] Previously, it was reported that photoionization of trans-stilbene occurs in solution via radical cation.[12-13] The ionization mechanism still remains controversial with an intriguing fact that the rise of the radical cation shows a marked delay from the photoexcitation.[7] Two most popular photoisomerization mechanisms of stilbene analogues in solution have been reported: a). One bond twist (OBT) mechanism, [14-16] b) Hula-twist (HT) mechanism. [17-19]

Photoisomerization may occur simply a homolytic or a heterolytic breaking of the C=C bond in solution.[8] Partially double bond character of C=C bond is observed by resonance and facilitates the interconversion. Exciplex-induced isomerization plays a key role in highly efficient photoisomerization of stilbene-cored dendrimer.[20-21] Eyring et al. had proposed two alternatives: isomerization either through the formation of a biradical (on a triplet surface) or in the ground state (S_0) by rotation about the C=C bond.[22] Buechele et al. suggested the formation of a transient intermediate through tautomerization during trans-cis isomerization for conjugated dienes.[23]

Recently, effect of substituents and solvent on photochemistry of stilbene analogues has been widely investigated for understanding the mechanism of photoisomerization process.[23-27] Stilbene and azobenzene analogues represent mostly studied cases of photoisomerization by both experimentally and theoretically.[28-31] Role of ground and excited state of molecule during photochemical process has been investigated widely by theoretical studies.[32-35] The state, geometry dependent and the shape of the $S_1(\pi\pi^*)$ potential energy curve (PEC) along the C=C torsion are important for better understanding the photoisomerization process of stilbene analogues. [36] Photocleavage of stilbene is observed in presence of oxygen. [37] Mechanistic studies and photodegradation of 2,5-dialkyloxyl-substituted para-phenylenevinylene oligomers by singlet oxygen is also reported. [38]

From computational and experimental evidences, evolution of a charge transfer state populated directly upon photoexcitation and non-radiative deactivation to the ground state are affected by the polarity of the solvents, play important role on photoisomerization and photochemistry. [39-40]

It is reported that the cyano-substituted group has been found to open a non-radiative decay mechanism related to the isomerization of the double bond via a crossing (conical intersection) of electronic states with distinct nature via the conical intersect (CI). [40] Recently, our group has reported the photodissociation kinetic of bis-2-benzylidenemalononitrile (BBM) in solutions and role of cyano group and solvents. [41] Further, role of solvents and photodissociation of C=C bond in bis-2-benzylidenemalononitrile (BBM) are not clearly understood.

In present work, we have investigated photochemistry and photodissociation of C=C bond in photoactive bis-2-benzylidenemalononitrile molecules (BBM, Chart 1). Solvent and environment dependency of photodissociation have been investigated throughout work. Interesting observations are obtained from our present work.

Experimental Section

UV-Vis Spectroscopy

Electronic absorption spectrum is measured on Varian-UV-Visible spectrophotometer (Carry-100-Bio) in various solvents and different aqueous CTAB solution. A 1 cm quartz sample cell at the rate of 0.5 °C/min during the heating and cooling scans using Cary 100-Bio UV-Vis spectrophotometer (Varian Carry-100-Bio) equipped with a Peltier series II thermostatic cell holder.

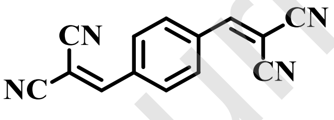
Synthesis of Bis-2-benzylidenemalononitrile (BBM)

Synthetic procedure of BBM was reported in our previously work. [42] In brief, a mixture of terephthaldehyde (1.0 mmol), manolonitrile (2.01 mmol) and MP(DNP) (0.05 mmol) in round bottom flask containing ethanol was stirred at room temperature for appropriate time. After completion of the reaction, which was monitored by TLC, the solid product was collected by filtration, washed with water and ethanol for obtaining pure product.

Characterization of BBM: State: Solid; Colour: White; Melting Point: 205 °C; FTIR (KBr, cm^{-1}): 2938, 2228, 1556, 1565, 1494; ^{1}H-NMR (300MHz, $CDCl_3$): δ (ppm) 8.04 (d, J = 7.0 Hz, 4H), 7.81 (s, 2H); ^{13}C-NMR (125 MHz, $CDCl_3$): δ (ppm) 160.3, 135.8, 131.3, 114.3, 113.2, 85.2; ESIMASS: [M+H] 231.2.

Sample Preparation

Time dependent UV-Vis spectra of BBM is measured under UV irradiation at 365 nm for 1 minute before and after during UV-Vis measurement in solvents. Commercially available 4-watt power of UV lamp @ 365 nm is exposed for 1 minute on the sample. The concentration of BBM is ~10^{-5}(M) in solvents during experiment.



Bis-2-benzylidenemalononitrile **(BBM)**

Chart 1: Structural Formula and Abbreviation

Results and discussion

Photodissociation kinetics of selective C=C bond in BBM is investigated in different micelle concentration at room temperature. Influence of hydrophobic and hydrophilic factors on rate of photodissociation (k) has also investigated.

Time Dependent UV-Visible Studies at Different Aqueous CTAB Micelles Concentration.

Time dependent UV-Vis study of BBM is carried out in different solvents for understanding the effect of solvents on photodissociation via solute-solvent interaction. In polar aprotic solvents, UV-Vis spectra of BBM is not changed under UV irradiation for 1 minute during time dependent UV-Vis studies but significant spectral variation is observed in polar protic solvents under same condition (ESI- Figure 1). So, photodissociation process is occurred during time dependent UV-Vis spectral measurement in protic polar solvents.

Interestingly, time dependent UV-Vis spectra and its spectral pattern in H_2O are different from other polar protic solvents and indicates special solute-H_2O interaction during photodissociation process. In time dependent UV-Vis spectra in H_2O, two isosbestic points are observed at 598 nm and 283 nm respectively during photodissociation reaction under UV irradiation (ESI-Figure 2). The kinetic of this photodissociation reaction is fitted with pseudo 1^{st} order kinetic model. The 1^{st} order kinetic model for photochemical process is considered and rate constant (k) is found to $\sim 10^{-3}$ s^{-1} in different protic solvents and binary solvent at 25 °C. The pseudo 1^{st} order rate constant (k) is calculated monitoring at 403 nm with time in H_2O and found to be $2.4\text{x}10^{-3}s^{-1}$. Similarly, pseudo 1^{st} order rate constant (k) is calculated monitoring at 348 nm with time in binary solvent (ACN-H_2O) and found to be $6.2\text{x}10^{-4}s^{-1}$ (ESI-Figure 3). Further, different alcoholic solvents, the rate constant (k) was also significantly different and found to be $4.4\text{x}10^{-4}s^{-1}$ for EtOH and $1.2\text{x}10^{-4}s^{-1}$ for 2-Pro-OH respectively.[41]

Generally, critical micelle concentration (CMC) of CTAB in H_2O is found to be 0.9 mM at room temperature. So, above 0.9 mM of aqueous CTAB solution, different micelle concentration of aqueous CTAB solution is formed. To investigate the rate of photodissociation under UV irradiation, time dependent UV-Vis study is carried out in different aqueous CTAB solution at room temperature. From time dependent UV-Vis spectra in 2.5 mM aqueous CTAB solution, one isosbestic point is observed at 304 nm during photodissociation reaction under UV irradiation (Figure 1). In UV-Vis spectra, longer wavelength region is not affected significantly (500-900 nm). The kinetic of this photodissociation reaction in 2.5 mM aqueous CTAB solution is fitted with pseudo 1st order kinetic model and rate constant (k) is found to be $1.1\text{x}10^{-3}$ s^{-1} at 25 °C.

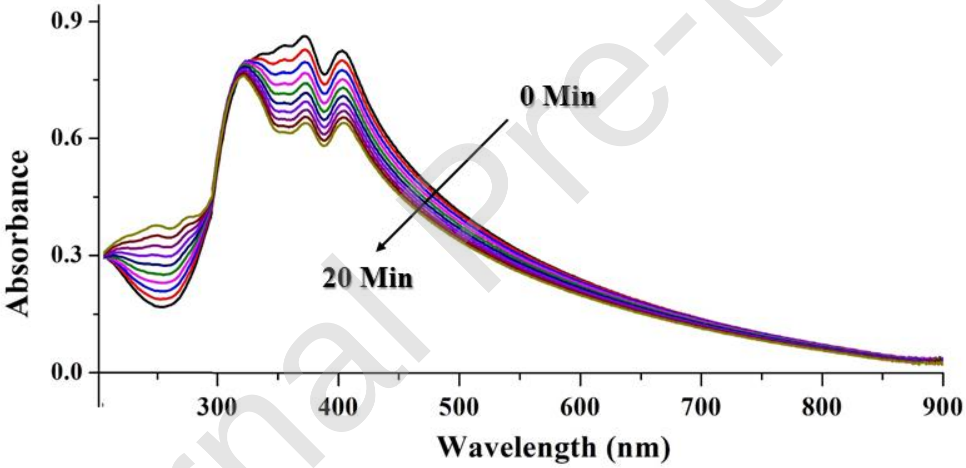


Figure 1. Time dependent UV-Vis spectra of BBM in 2.5 mM aqueous CTAB solution (External UV Irradiation at 365 nm for 1 minute during UV-Vis measurement)

Similarly, one isosbestic point is observed at 295 nm during photodissociation reaction under UV irradiation in 5 mM aqueous CTAB solution from time dependent UV-Vis spectra (Figure 2). In UV-Vis spectra, longer wavelength region is affected significantly (350-900 nm). The kinetic of this photodissociation reaction in 2.5 mM aqueous CTAB solution is fitted with pseudo 1st order kinetic model and rate constant (k) is found to be $2.1x10^{-3}$ s^{-1}.

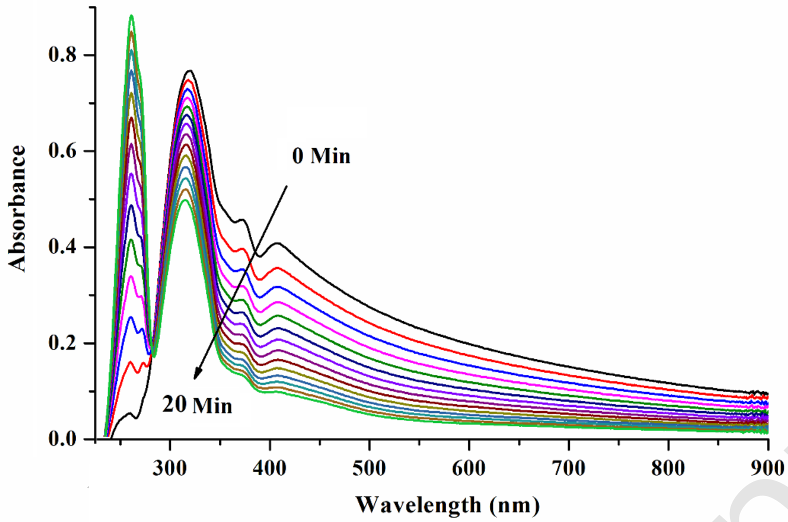


Figure 2. Time dependent UV-Vis spectra of BBM in 5 mM aqueous CTAB solution (External UV Irradiation at 365 nm for 1 minute during UV-Vis measurement)

Further, one isosbestic point at 295 nm is observed under UV irradiation in 10 mM aqueous CTAB solution from time dependent UV-Vis spectra (Figure 3). In UV-Vis spectra, longer wavelength region is disappeared (350-900 nm) with time and affected significantly. The kinetic of this photodissociation reaction in 10 mM aqueous CTAB solution is fitted with pseudo 1st order kinetic model and rate constant (k) is found to be $5.6x10^{-3}$ s^{-1}. With increase of aqueous CTAB concentration, value of specific rate constant (k) increases two-fold when concentration of aqueous CTAB solution is doubled.

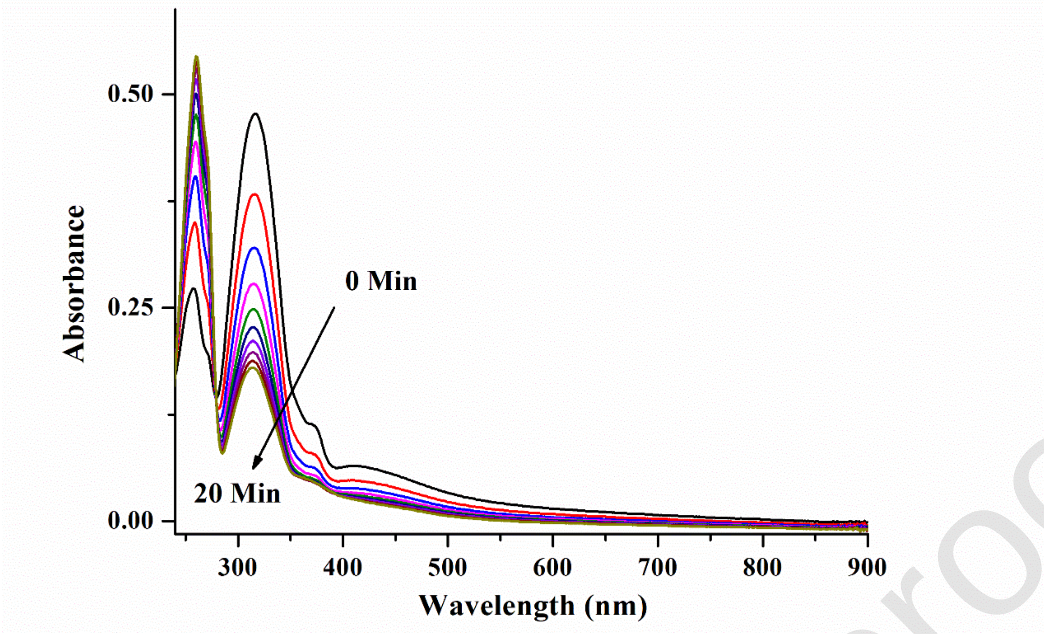


Figure 3. Time dependent UV-Vis spectra of BBM in 10 mM aqueous CTAB solution (External UV Irradiation at 365 nm for 1 minute during UV-Vis measurement)

In 50 mM aqueous CTAB solution, four isosbestic points are observed at 405, 348, 277 and 240 nm respectively under UV irradiation from time dependent UV-Vis spectra (Figure 4). In UV-Vis spectra, longer wavelength region is disappeared (350-900 nm) with time. The kinetic of this photodissociation reaction in 50 mM aqueous CTAB solution is fitted with pseudo 1st order kinetic model and rate constant (k) is found to be 10x10^{-3} s^{-1}.

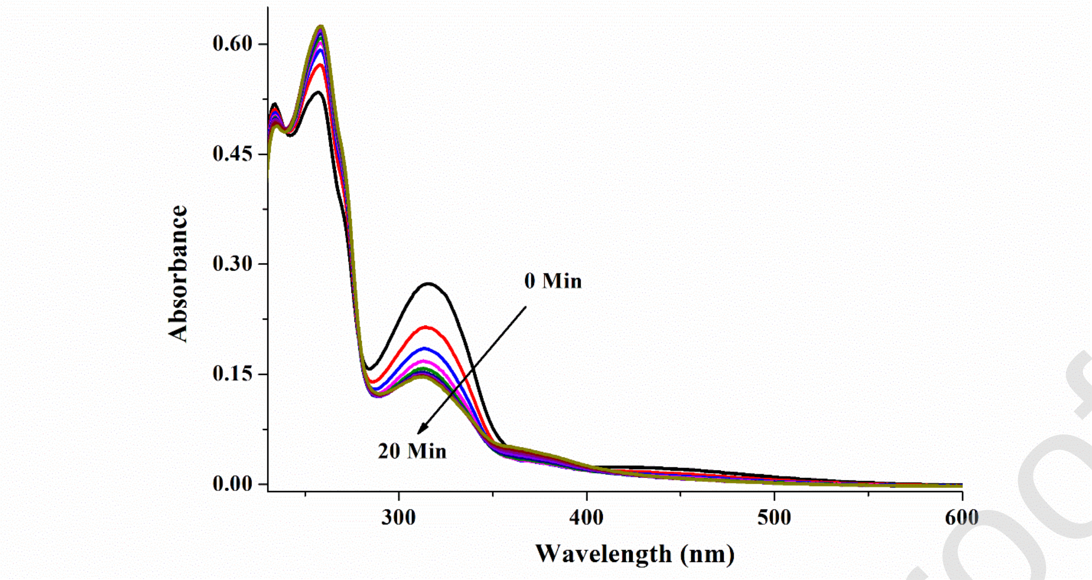


Figure 4. Time dependent UV-Vis spectra of BBM in 50 mM aqueous CTAB solution (External UV Irradiation at 365 nm for 1 minute during UV-Vis measurement)

The variation of rate constant (k) is plotted with different concentered aqueous CTAB solution in Figure 5 and presented in Table 1. Interesting factor is that the rate constant (k) is not further enhanced with increase of CTAB concentration up to 100 mM solution.

Table 1: Calculated rate constant (k) in different CTAB micelle concentration at 25 °C

	2.5 mM @ CTAB	5 mM @ CTAB	10 mM @ CTAB	50 mM @ CTAB	100 mM @ CTAB	2.5 mM @ KCl
k (s^{-1})	$1.1x10^{-3}$ @ 403 nm	$2.1x10^{-3}$ @ 403 nm	$5.6x10^{-3}$ @ 315 nm	$10x10^{-3}$ @ 315 nm	$10x10^{-3}$ @ 315 nm	$2.2x10^{-3}$ @ 403 nm
χ^2	0.99	0.99	0.99	0.99	0.99	0.99

Change of rate constant (k) with variation aqueous CTAB concentration has been analyzed using curve fitting method. We have fitted the experimental results with exponential growth profile and found that the increasing rate of rate constant (k) with variation of aqueous CTAB concentration is 0.09 with χ^2 = 0.98 (Figure 5). The specific rate constant (k) of photodissociation is observed maxima at 25 mM CTAB solution. The rate constant (k) is increased at different concentration of aqueous CTAB solution and higher compared to solvents at room temperature. But above concentration of aqueous CTAB (> 50 mM), rate constant (k) is almost constant and found to be 10×10^{-3} s^{-1} (Figure 5).

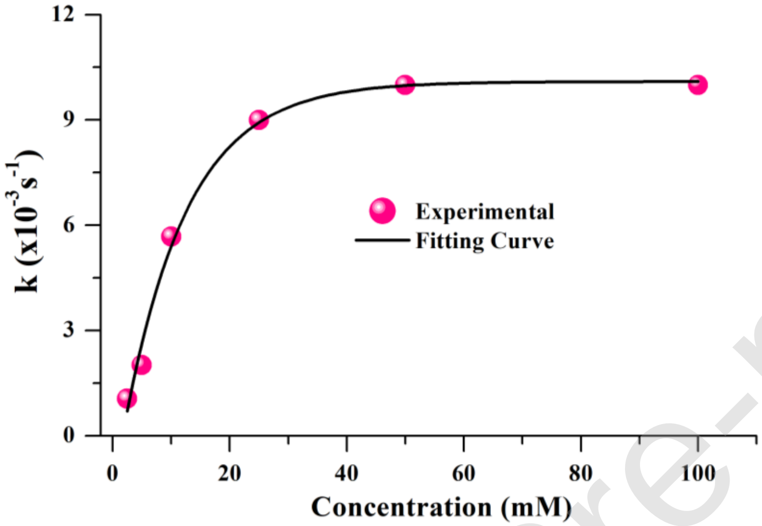


Figure 5: Variation of rate constant (k) with different aqueous CTAB solution

To investigate the effect of ionic strength on photodissociation process, different concentrated aqueous KCl solution is used. It is observed that concentration of aqueous KCl solution cannot influence on rate of photodissociation at room temperature (ESI-Figure 4-5).

From above experimental results, it is clear that ionic environment (in presence of aqueous KCl) does play important role on photodissociation kinetics but different micelle concentration plays significant role on enhancement of photodissociation kinetics. In micelle, hydrophobic region plays important role on enhancing rate of photodissociation. Considering above experimental facts, we have proposed a mechanism of photodissociation process in micelle environment and presented in Figure 6.

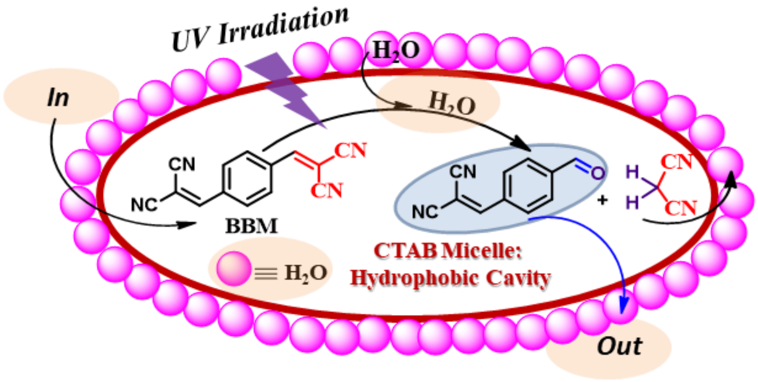


Figure 6: Mechanism of photodissociation process in micelle environment

In micelle environment, BBM molecules entered to hydrophobic cavity of micelle and reacts with water photodissociation occurred. Photo-dissociated product is coming out from hydrophobic cavity. At higher micelle concentration, large number of hydrophobic cavities would be available and density of BBM molecule in hydrophobic cavity of a micelle would be higher, results enhancement of photodissociation process.

Conclusion

In conclusion, photodissociation kinetics of selective C=C bond in BBM is investigated in different micelle concentration. In polar protic and polar aprotic solvents, rate of photodissociation (k) is significantly lower compared to H_2O solvent at room temperature. But interesting factor is that rate of photodissociation (k) is enhanced with increasing aqueous CTAB concentration and found to be highly sensitive to aqueous CTAB concentration.

From experimental results, it is clear that ionic environment (in presence of aqueous KCl) does play important role on photodissociation kinetics but different micelle concentration plays significant role on photodissociation kinetics. In micelle, hydrophobic region plays important role on enhancing rate of photodissociation. The rate of photodissociation is highest at 25 mM aqueous CTAB solution and found to be $10x10^{-3}s^{-1}$, which is five-fold higher than H_2O (k =

$2.0x10^{-3}s^{-1}$) at room temperature. It can be stated that rate of photodissociation in hydrophobic environment (specially CMC condition) is higher compared to polar protic and aprotic solvents.

ASSOCIATED CONTENT

Supporting Information

This material is available free of charge via the Internet at ***http://***

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1. Conflict of Interest

No conflict of interest exists.

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Notes

The authors declare no competing financial interest

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