Dynamical behavior of probe molecules and dominant role of cosurfactants in reverse micelles

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Abstract

Reverse micelles (RM) are nanopools of water surrounded by surfactant molecules in a non-polar solvent. Our studies investigated properties of RM probe molecules in the interfacial boundary between water and non-polar solvents. Reichardt's dye, a probe molecule, was used to uncover properties of RM. UV/vis spectroscopy of Reichardt's dye reveals information about polarity and the dye's approximate residential location and also helps confirm molecular orbital energy diagram. We discovered an interesting phenomenon with Reichardt's dye in RM. Surprisingly, the UV/vis spectrum of Reicahrdt's dye in CTAB RM with octanol as a cosurfactant exhibits decreasing absorbance and a blue shift. Reichardt's dye in solely octanol shows an irreversible color change and similar UV/vis spectrum. Consequently, we conclude that Reichardt's dye resides near the interfacial layer/solvent boundary. Other cosurfactants do not result in the time dependent behavior suggesting a more dynamic interaction between octanol and Reichardt's dye.

Introduction

Reverse micelles are nanopools of water surrounded by surfactant molecules in a non-polar solvent. Our studies investigated properties of reverse micelles with cosurfactants in the interfacial boundary between water and the non-polar solvent. Reverse micelles have been widely investigated for years as a drug delivery media. Reichardt's dye is very sensitive to polarity changes to its environment. Therefore, it has been popular probe because of its solvatochromic properties. We chose it to elucidate subtle changes in our reverse micelle systems. This particular poster focuses in determining where in the system Reichard's dye resides on what causes the time dependent absorption behavior we observed.

Materials and methods

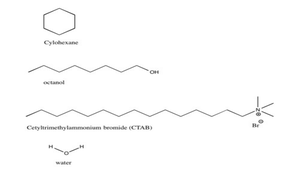


Figure 1: reverse micelles components: cyclohexane, octanol, CTAB and water

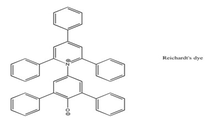


Figure 2: The structure shown above is Reichardt's dye, a probe molecule, to test the properties of reverse micelles.

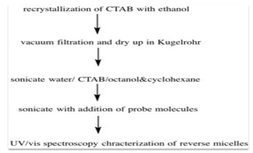


Figure 3: procedure to make reverse micelles

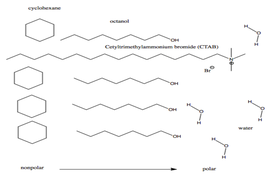


Figure 4: Materials to make reverse micelles. From left to right, layering from nonpolar to polar.

Results

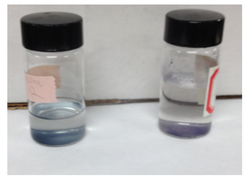


Figure 5: left: Reichardt's dye in water, right: Reichardt's dye in cyclohexane. They both have very faint color with most of the dye in the solid phase on the bottom.

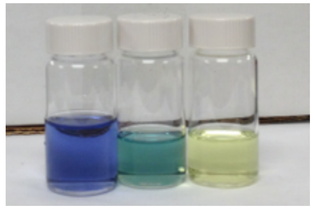


Figure 7: The figure above shows Reichardt's dye in 1-octanol demonstrating an irreversible color change from left to right. The dark purple solid when dissolved changed to blue in less than a minute and took about 5 minutes to turn from blue to green and another 10 minutes to become yellow from green.

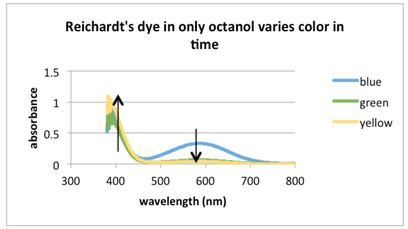


Figure 8: The spectra above are of Reichardt's dye dissolved in 1-octanol. The spectra are of the solutions in Figure 7. As the solution changes from blue to yellow the peak near 580 nm decrease and near 400 nm increases.

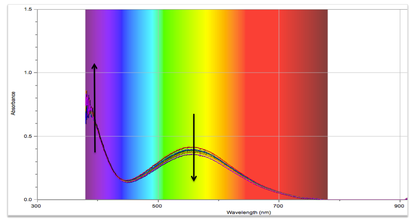


Figure 6: UV/ vis spectrum of CTAB reverse micelles with 1-octanol as a cosurfactant, cyclohexane as a solvent and Reichardt's dye as the probe molecule.

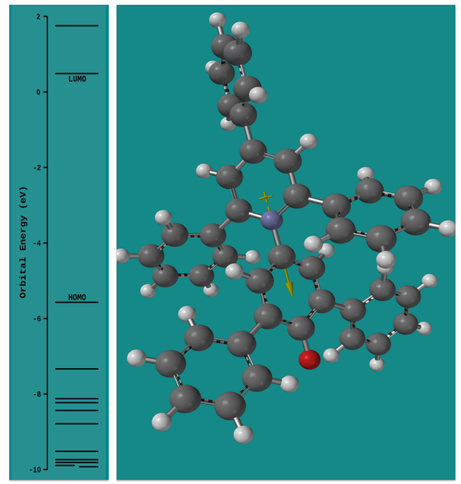
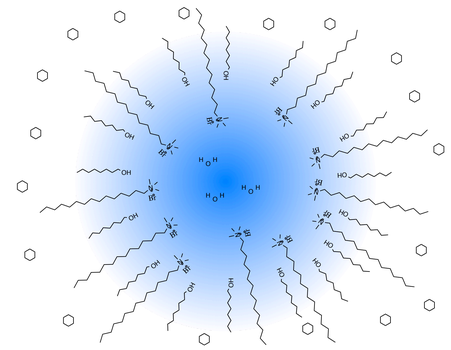


Figure 9: Three dimensional representation of Reichardt's dye illustrating its Christmas tree-like structure along with its molecular orbital energy diagram. The Spartan molecular orbital diagram was generated at equilibrium geometry at ground state with Hartree-Fock level of calculation with a 3-21 G basis set. The benzene rings are not planar relative to one another and the direction of dipole points toward oxygen.

What do reverse micelles look like?



Conclusions

Evidence suggested that

- Reichardt's dye does not reside in cyclohexane and water because there is no evident peak in solely cyclohexane or water with Reichardt's dye.
- Reichardt's dye resides near the interfacial layer/solvent boundary.
- Subtle and slow environmental changes depend on the presence of 1-octanol .
- Corrigan[1] et al, data show similar behavior for Reichardt's dye in 4-chloro-1-butanol and attribute that behavior to a methylation reaction. However, that does not explain the behavior we see because there is no halogen attached when we have only 1-octanol present. We suspect the behavior in RM more closely mimics the behavior in 1-octanol than Corrigan[1] proposes.

Further studies

- Refine computational studies of the molecular orbital energy diagram in first excited state.
- Compare behavior of Reichart's dye in AOT reverse micelles.

Literature cited

1. Corrigan, K. Damion; Whitcombe, J. Michael; McCrossen, Sean and Piletsky, Sergey. *Journal of pharmacy and Pharmacology. 2009, 61, 533-539.*

Acknowledgments

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