3. SANS Research Topics

A- Phase Transitions in Pluronic P85 Solutions

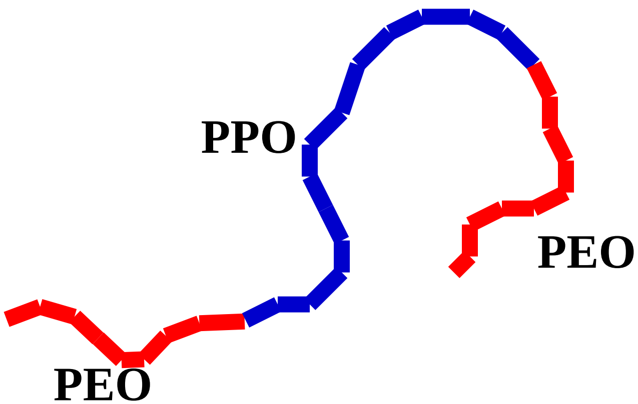
B- Polymer Co-solvation and Co-nonsolvation

C- SDS Micelles with Ethanol Co-surfactant

A - Phase Transitions in Pluronic P85 Solutions

Pluronics

Dissolved Unimer
(low temperature)

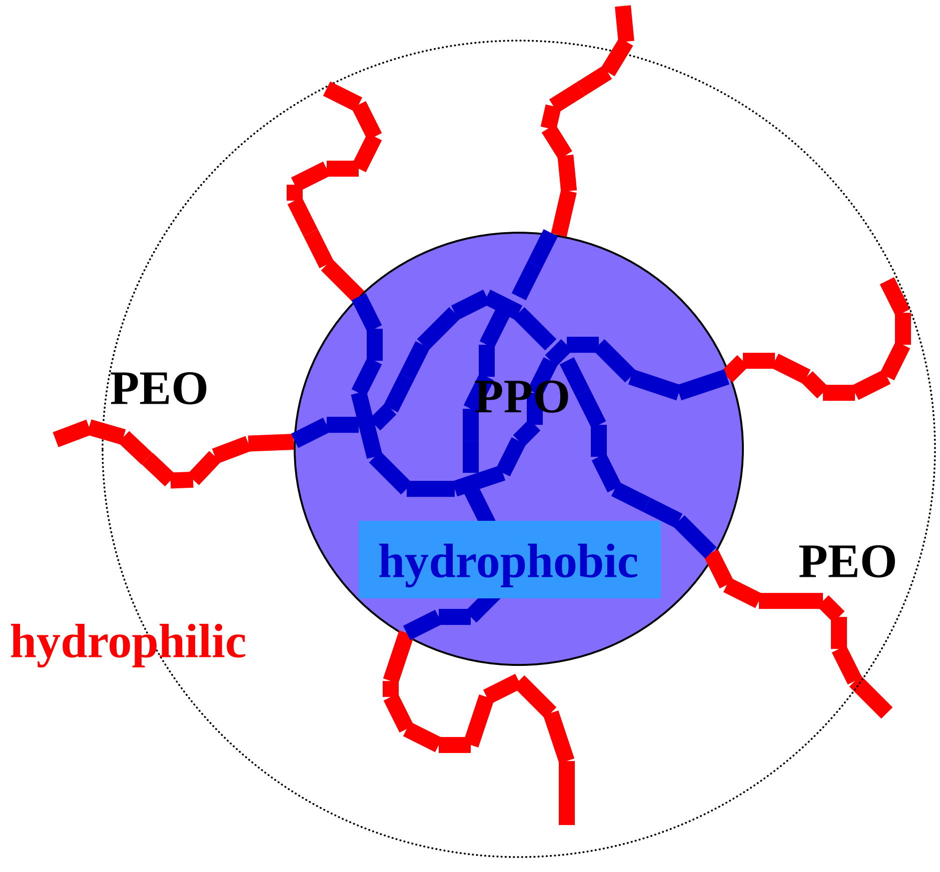


EO:$-CH_2CH_2-O-$

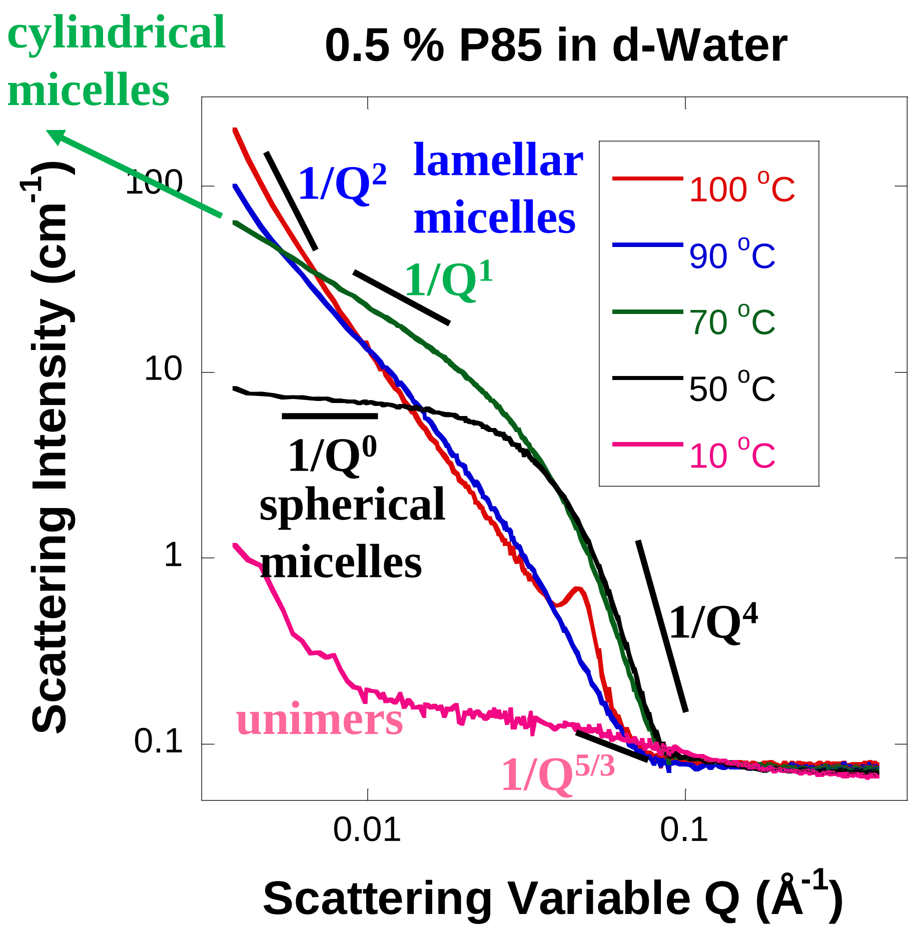
PO:$-CH(CH_3)CH_2-O-$

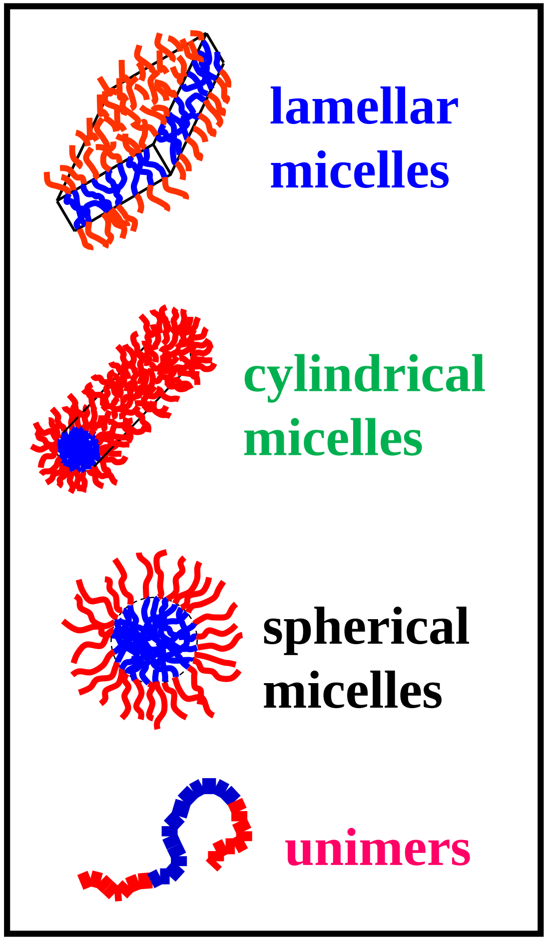
P85: $EO_{26}PO_{40}EO_{26}$

Formed Micelle
(high temperature)

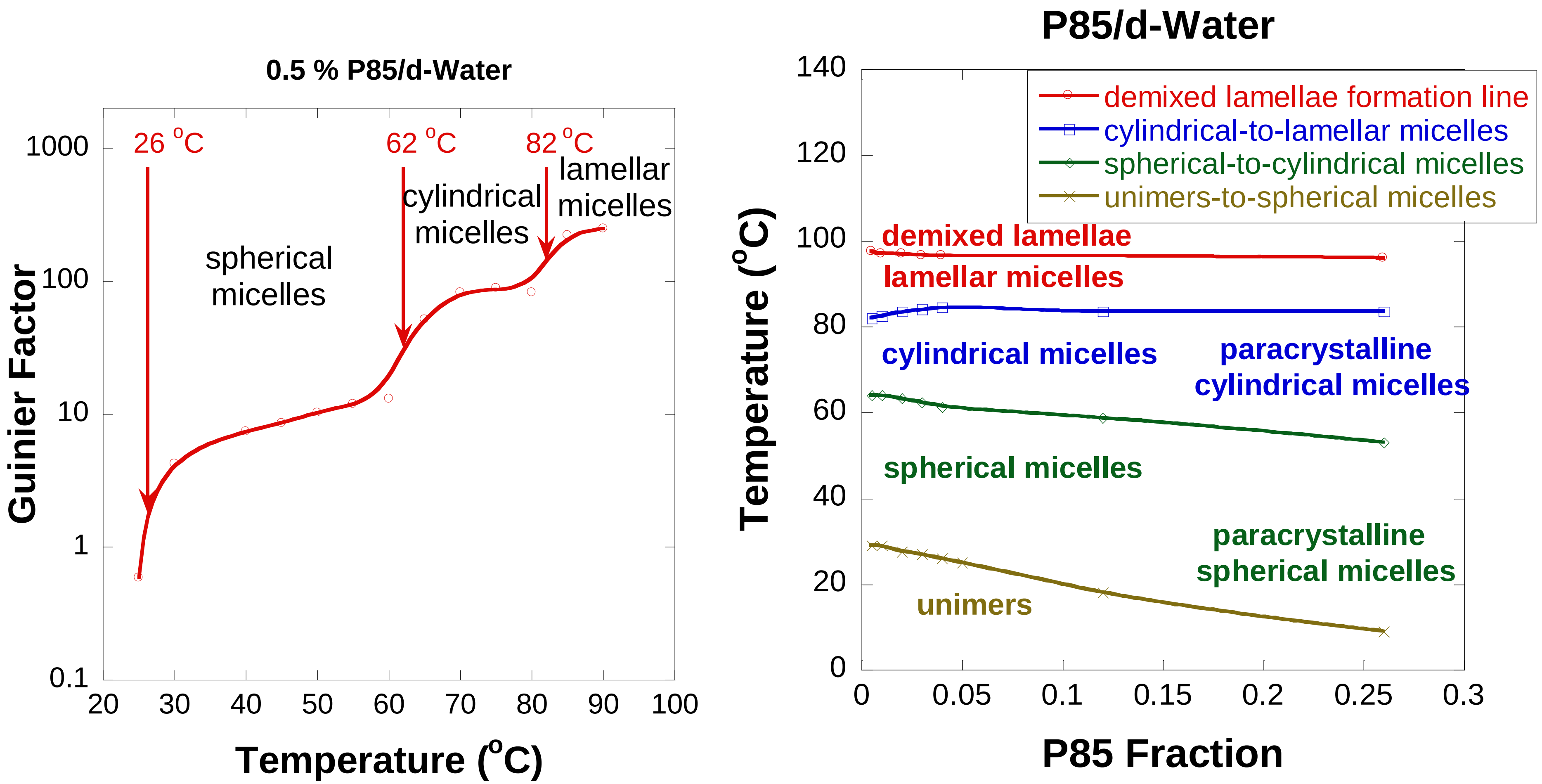


Pluronic Micelles





Phase Diagram

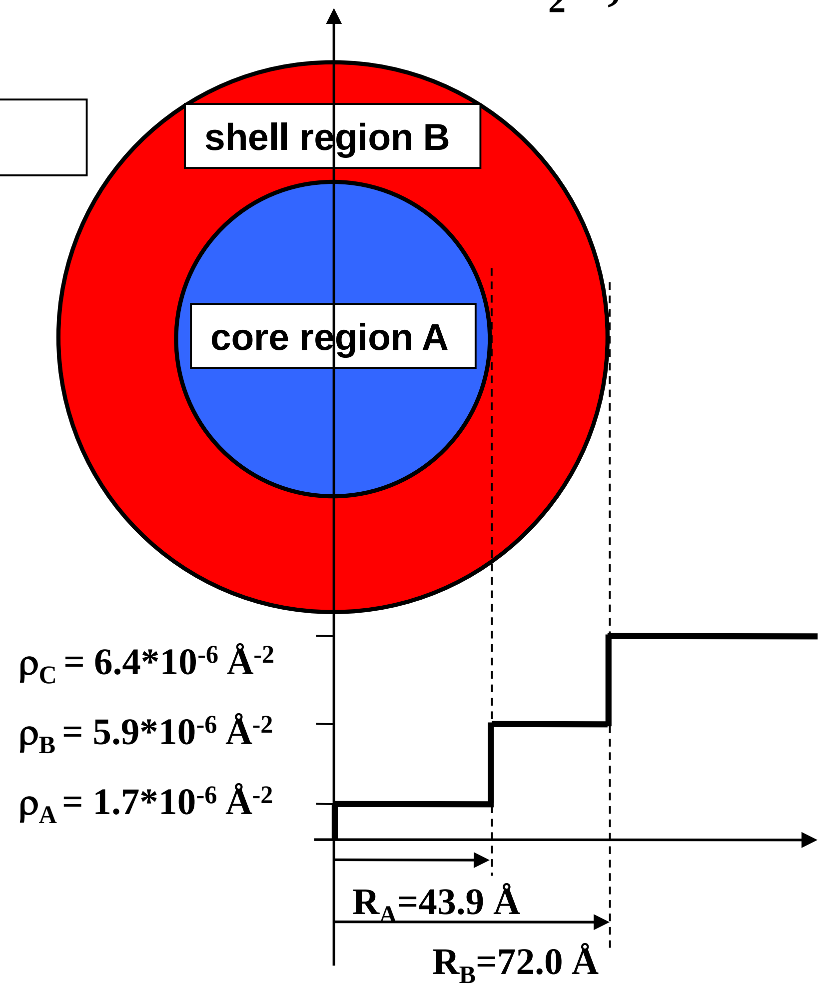


The Core-Shell Particles Model

$$\frac{d\Sigma(Q)}{d\Omega} = \frac{N}{V}\left[(\rho_A - \rho_B)V_A \frac{3j_1(QR_A)}{QR_A} + (\rho_B - \rho_C)V_{A+B}\left(\frac{3j_1(QR_B)}{QR_B}\right)\right]^2 S_I(Q)$$

10% P85 Pluronic/D_2O, 40 °C

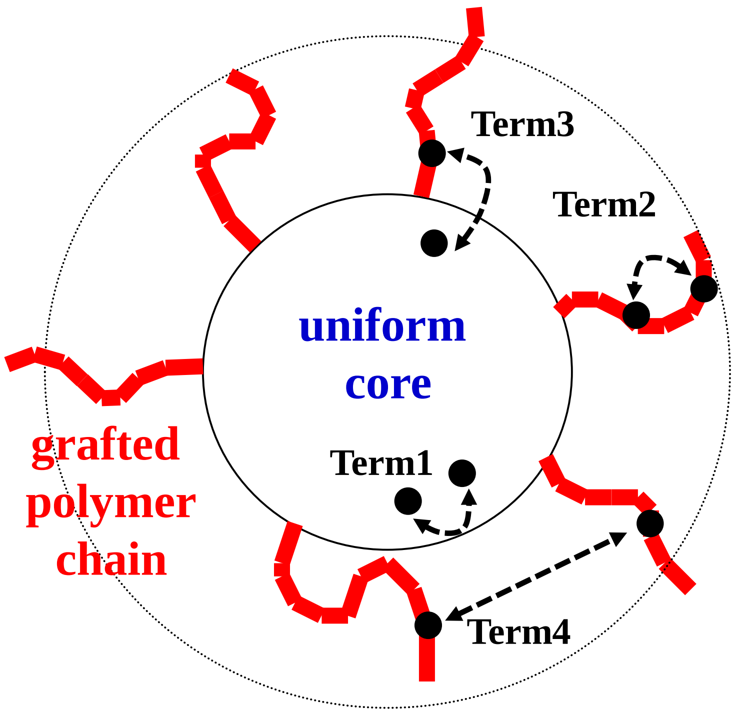
solvent region C



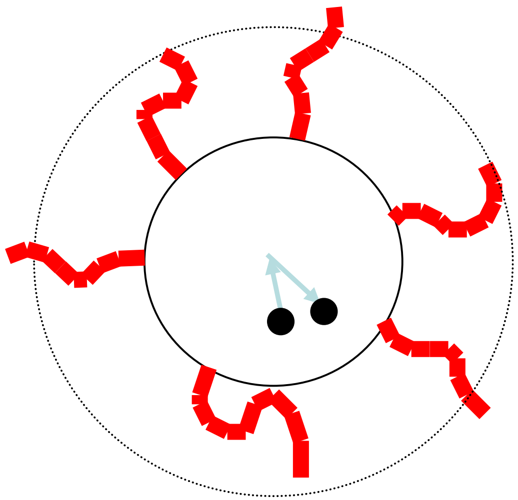
Fits yield

$\rho_C = 6.4 \times 10^{-6}$ Å^{-2}, $\rho_B = 5.9 \times 10^{-6}$ Å^{-2}, $\rho_A = 1.7 \times 10^{-6}$ Å^{-2}, $R_A = 43.9$ Å, $R_B = 72.0$ Å

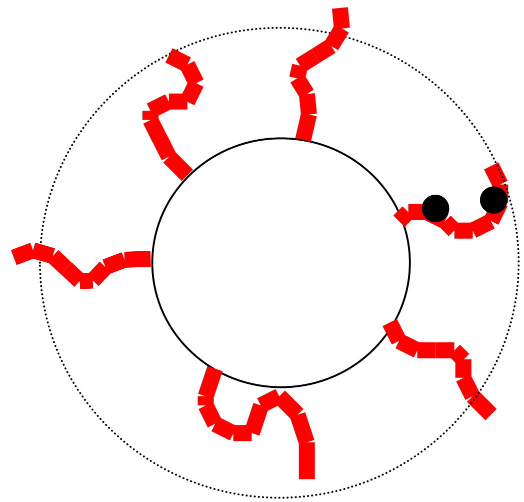
The Core-Chain Model



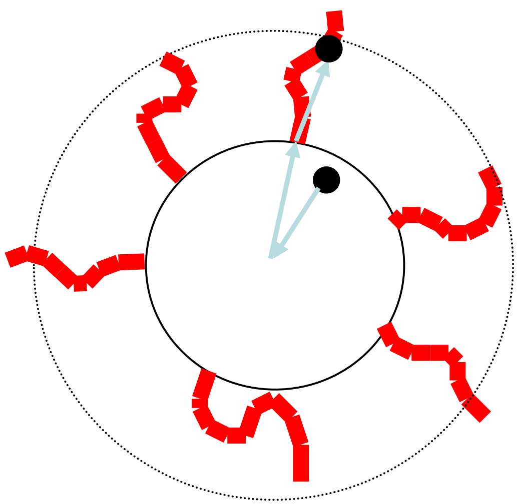
The Core-Chain Form Factors



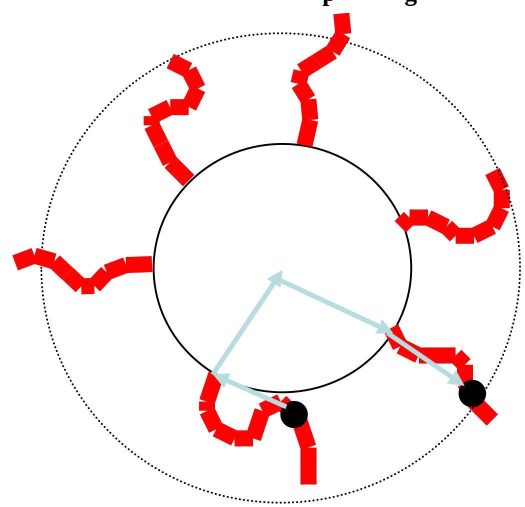
Term1=$P_c(QR)=F_c^2(QR)$



Term2= $P_p(QR_g)$



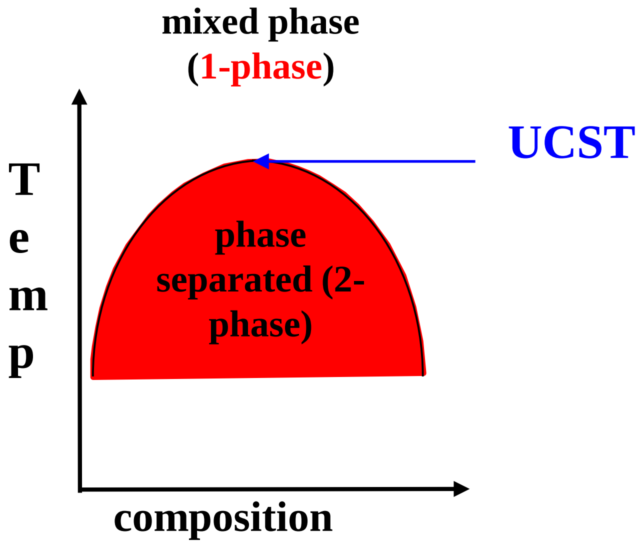
Term3= $F_c(QR)\ E_c(QR)F_p(QR_g)$



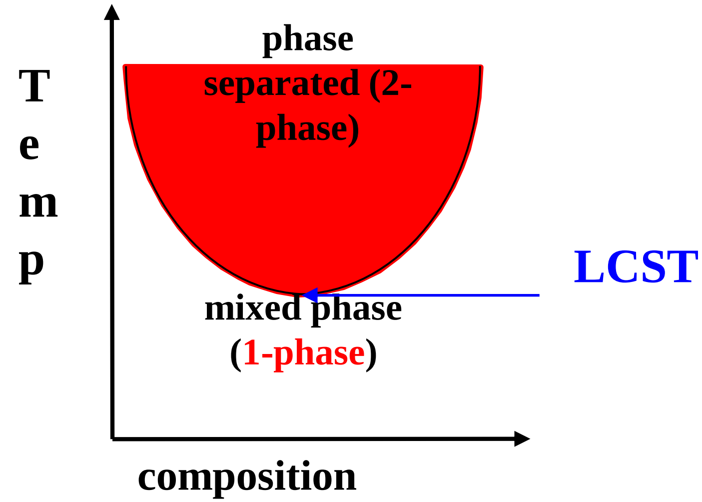
Term4= $F_p(QR_g)\ E_c^2(QR)F_p(QR_g)$

C- Polymer Co-solvation and Co-nonsolvation

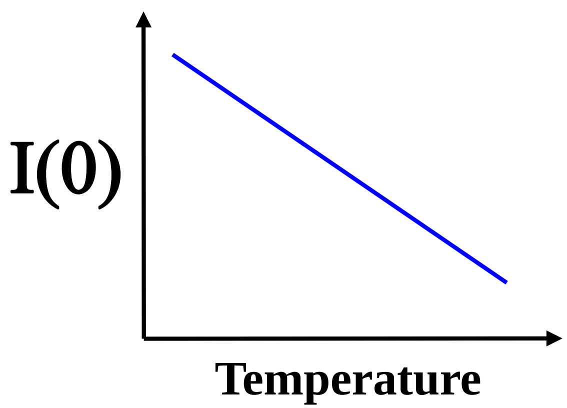
Polymer Demixing Phase Transitions

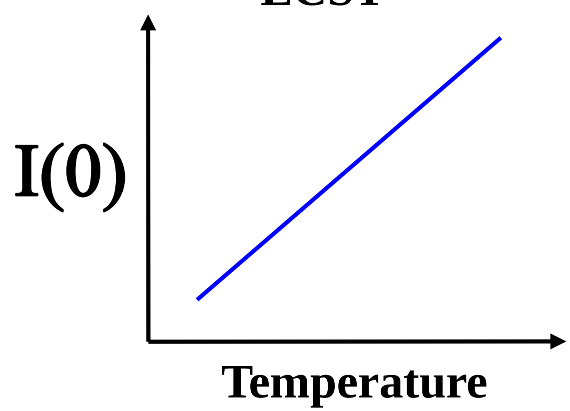


UCST



LCST

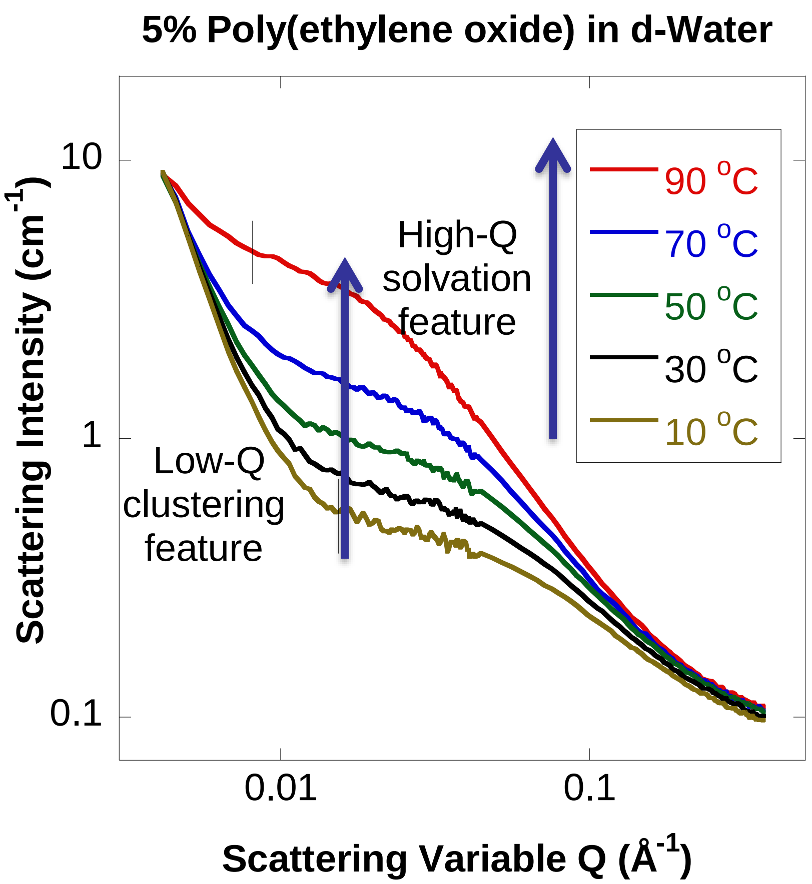




Upper Critical Solution Temp.

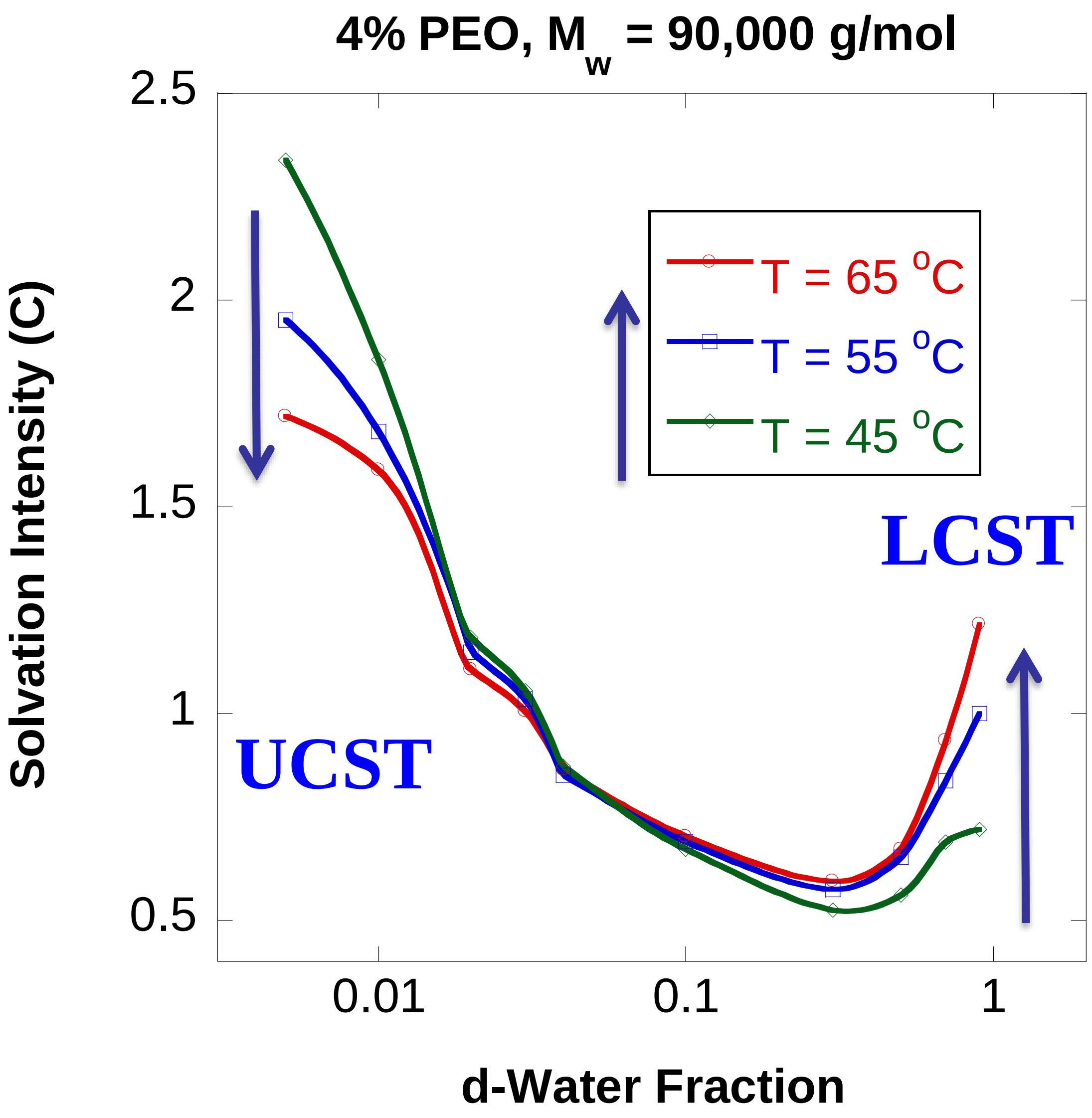
Lower Critical Solution Temp.

Poly(ethylene oxide) in d-water

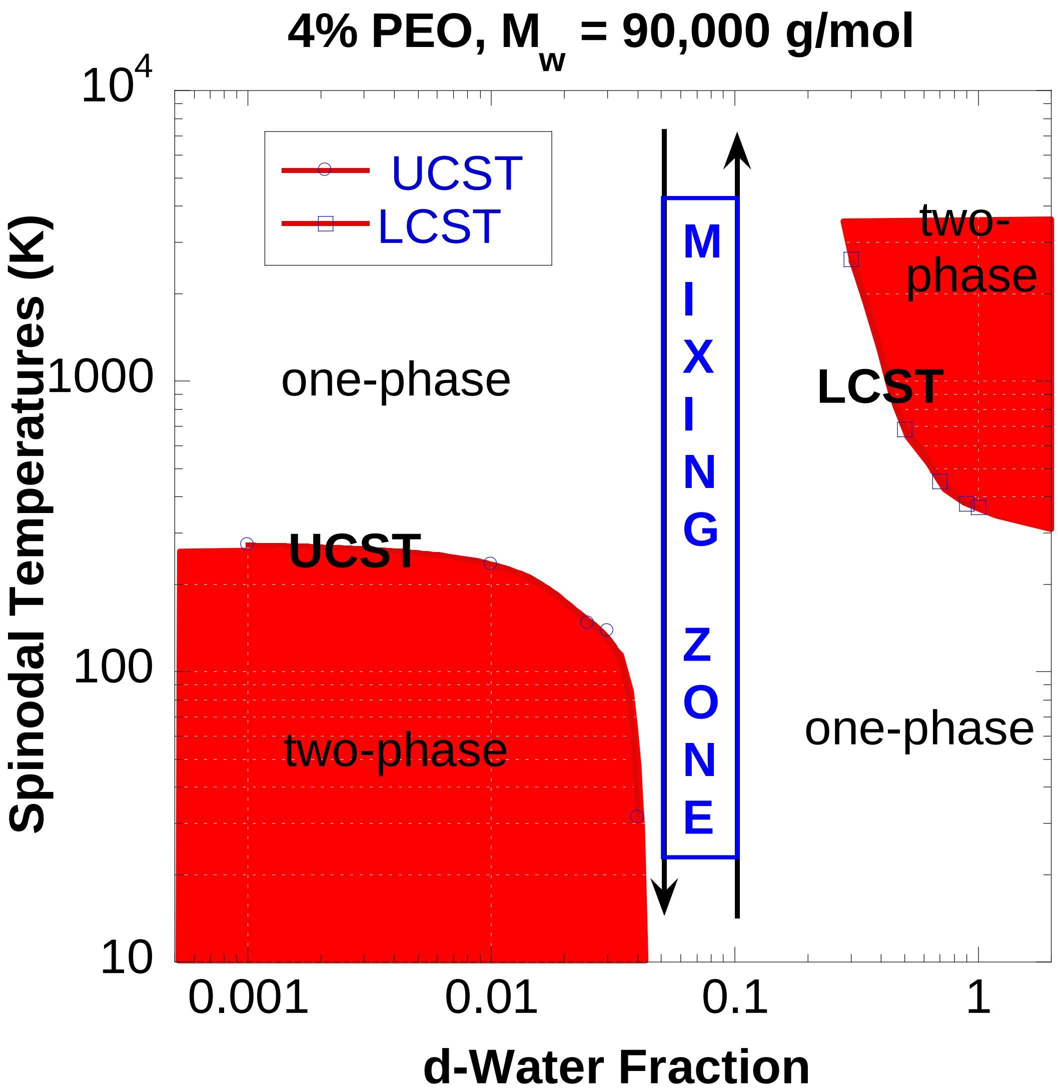


Lower Critical Spinodal Temperature

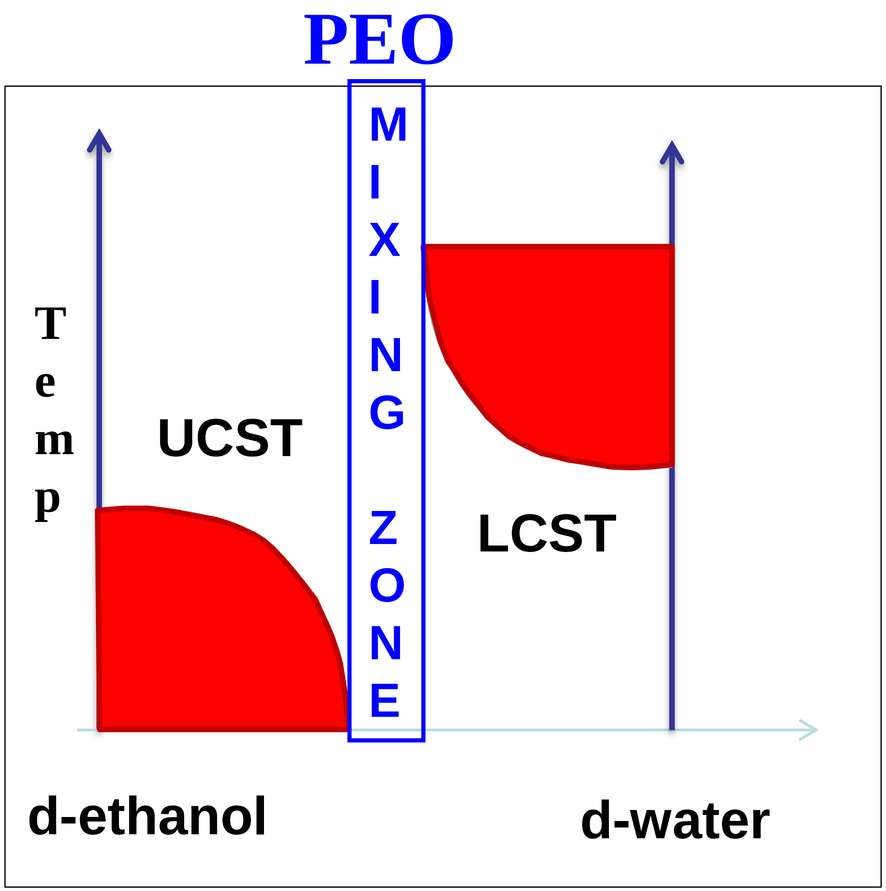
PEO in d-ethanol/d-water Mixtures

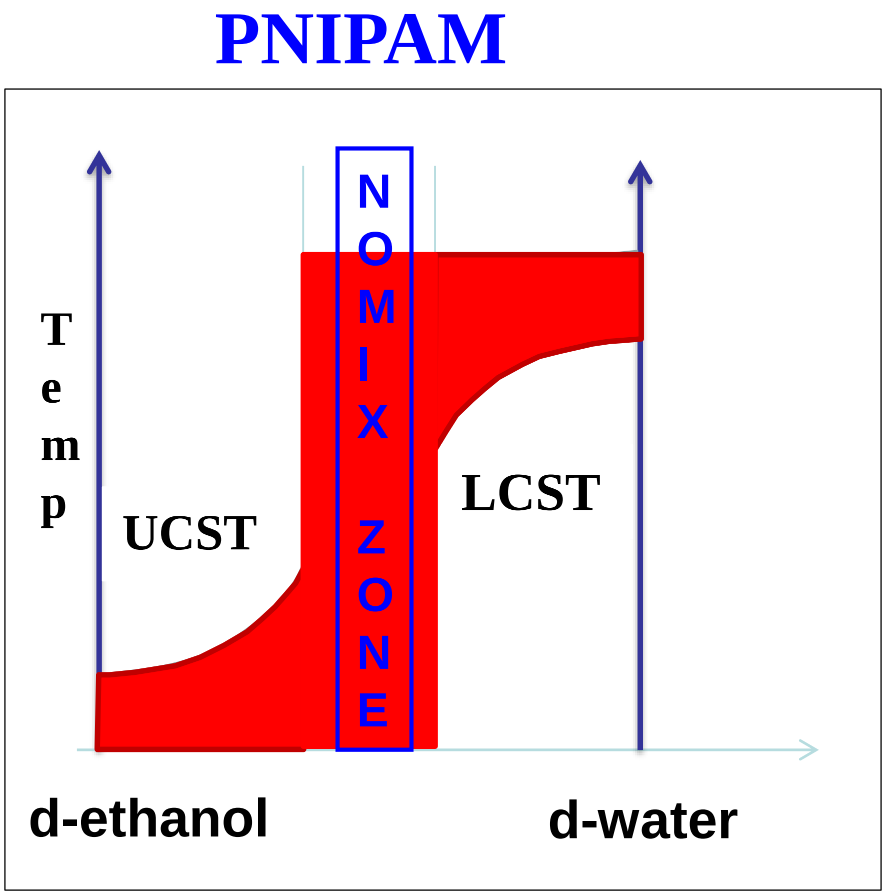


PEO in d-ethanol/d-water Mixtures



Co-solvation and Co-nonsolvation

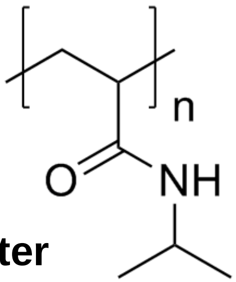


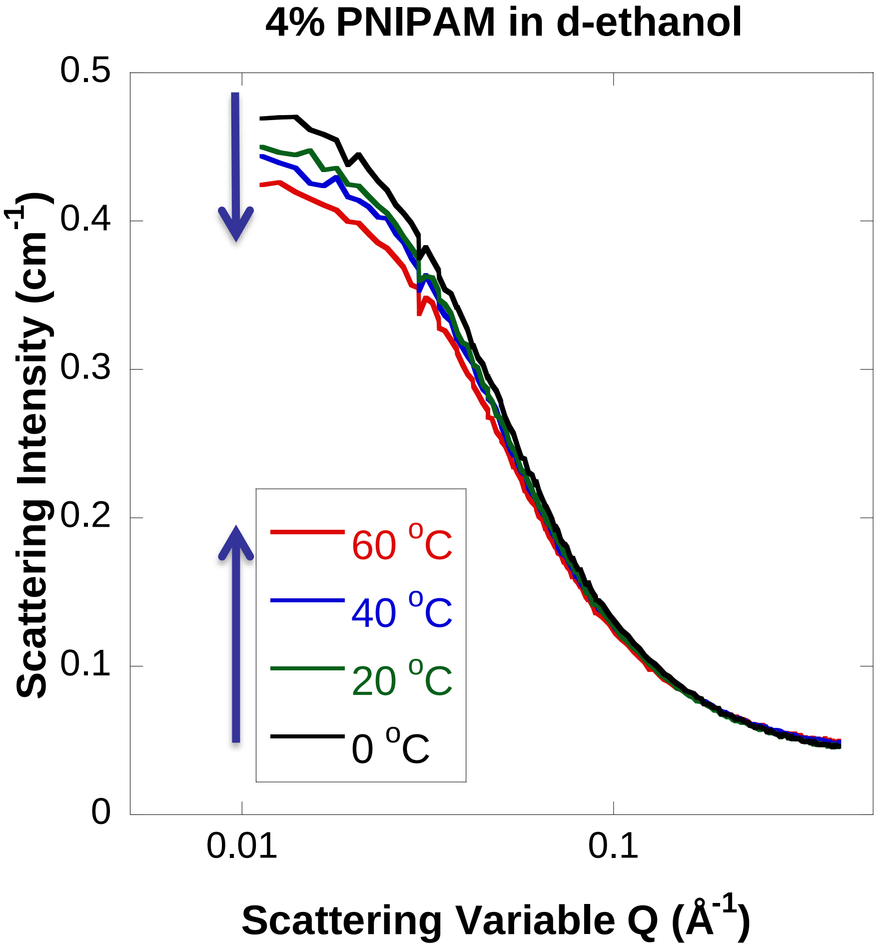


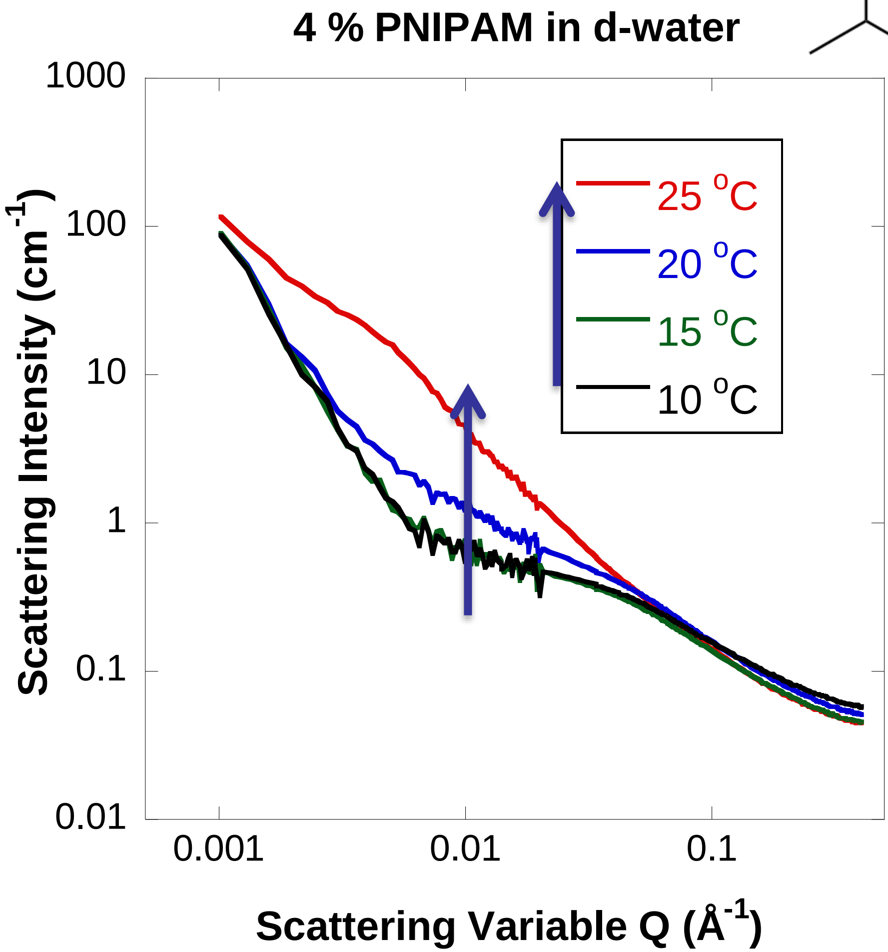
Co-solvation

Co-nonsolvation

PNIPAM in d-ethanol/d-water Mixtures



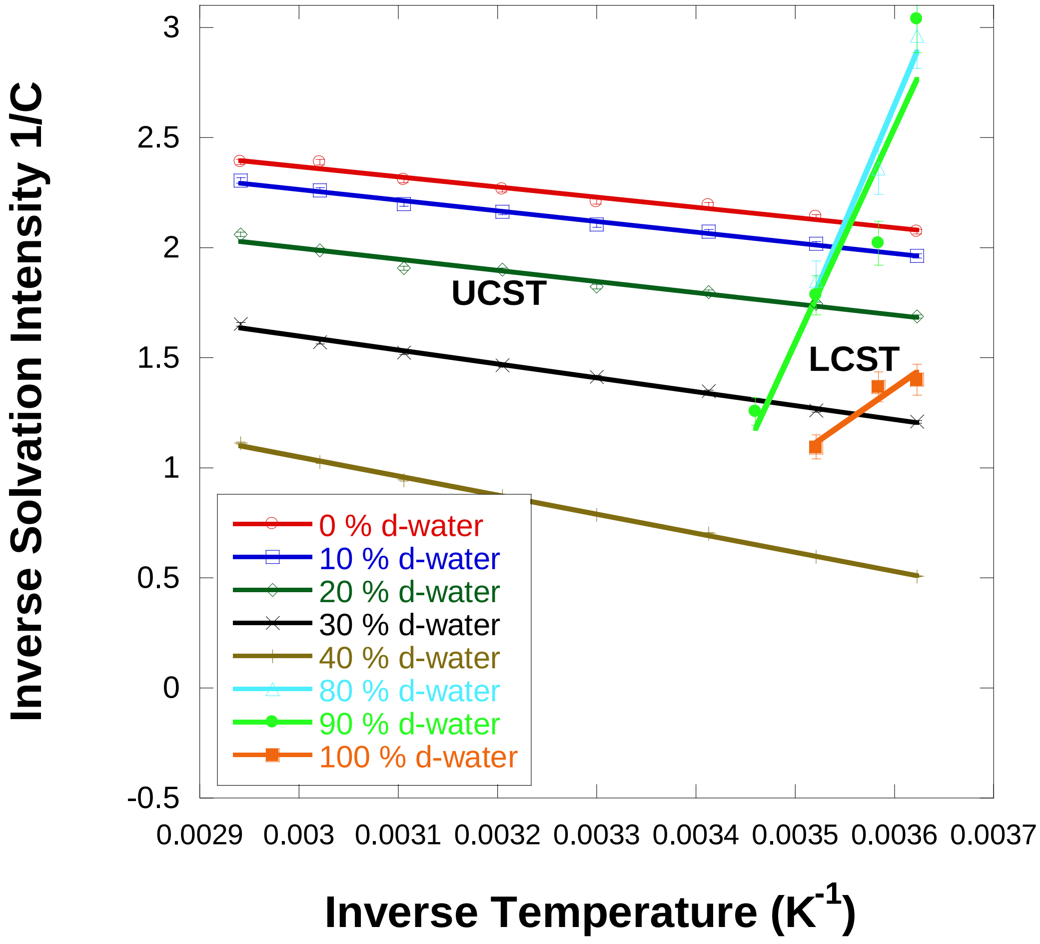




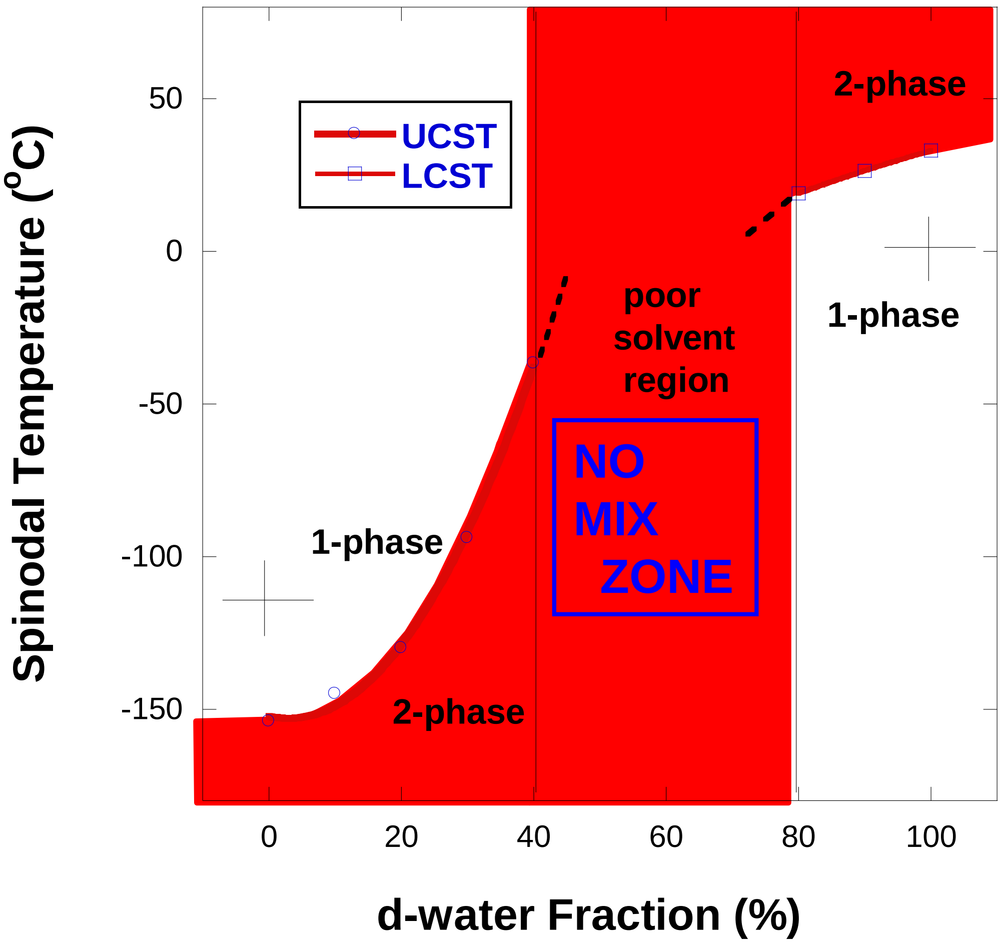
UCST

LCST

PNIPAM in d-ethanol/d-water Mixtures



PNIPAM in d-ethanol/d-water Mixtures



Results

- Most polymers dissolve better in solvent mixtures (cosolvation)

- PNIPAM obeys a co-nonsolvation rule

- PEO is characterized by a “perfect” solvation window for 10 % d-water.

- PEO dissolves in water while PMO and PPO do not dissolve.

- Water and water-ethanol mixtures form cage-like structures.

- PNIPAM is characterized by a non-solvation window for 60 % d-water.

- SANS is a valuable thermodynamic probe to study phase transitions as well as nanostructures

C- SDS Micelles with Co-surfactant

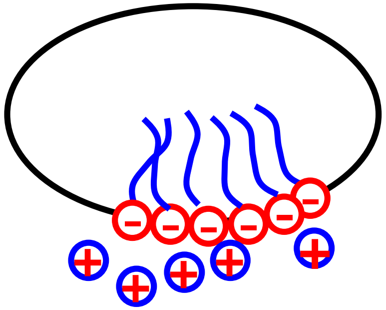
Micelle Formation

- **Surfactants are formed of a hydrophilic head and a hydrophobic tail**

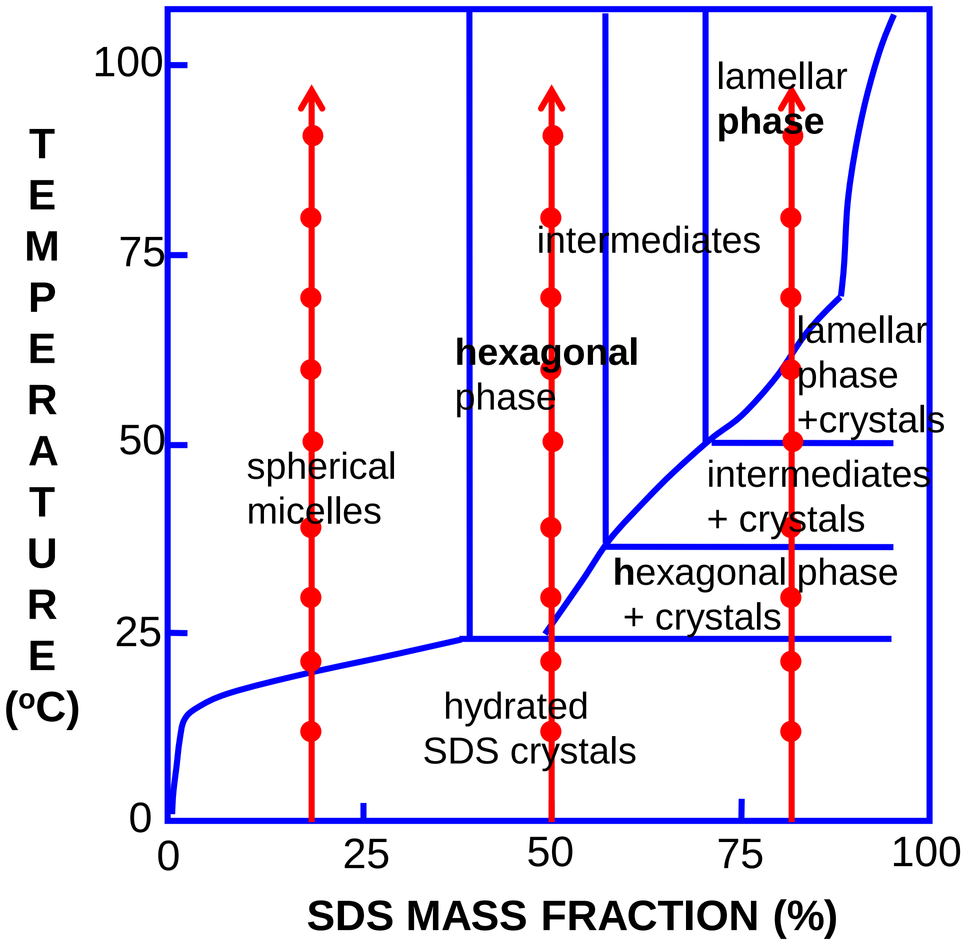
- **Micelles form when enough surfactants aggregate (above the critical micelle concentration or CMC)**

- **SDS surfactants form micelles in water (or deuterated water)**

- **What is the effect of ethanol co-surfactant on SDS micellar structure**

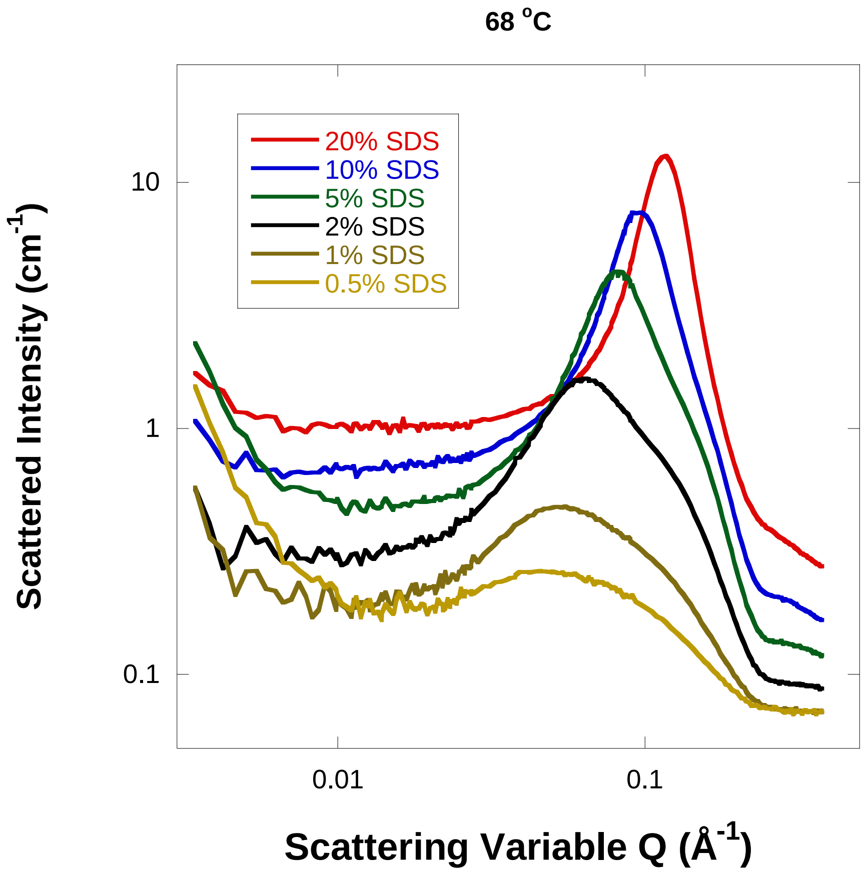


Phase Diagram

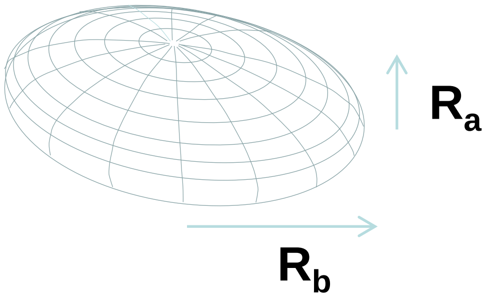


- SDS/water phase diagram from calorimetry

SANS from SDS Micelles

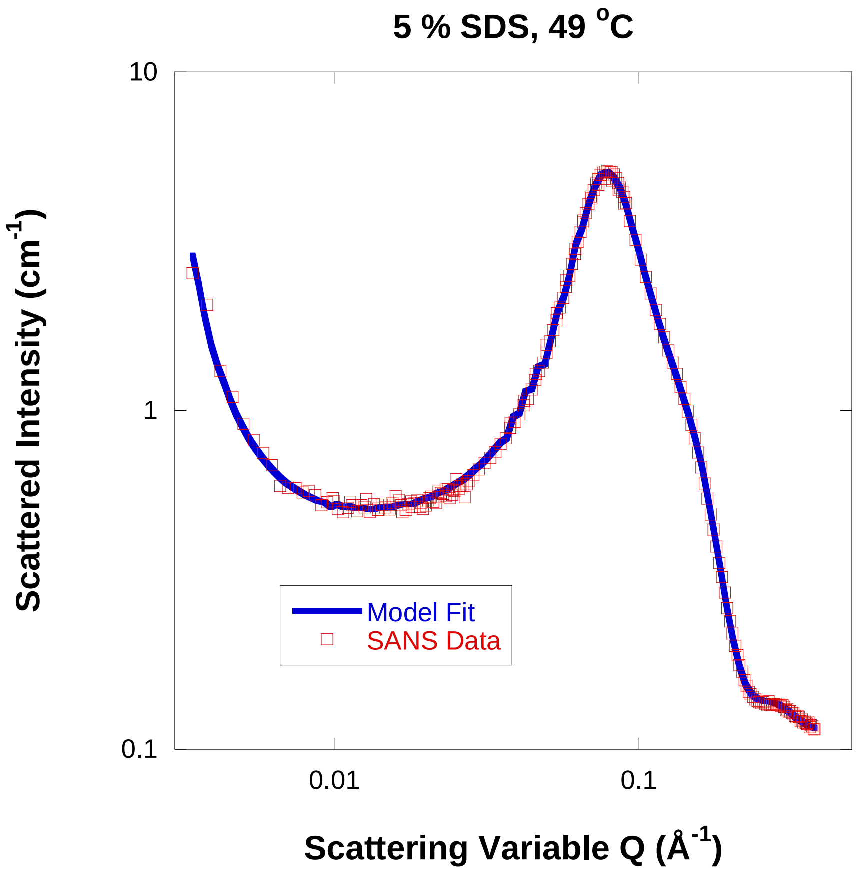


Oblate ellipsoid



- Ellipsoidal micelles form

Ellipsoid Micelles Model Fit

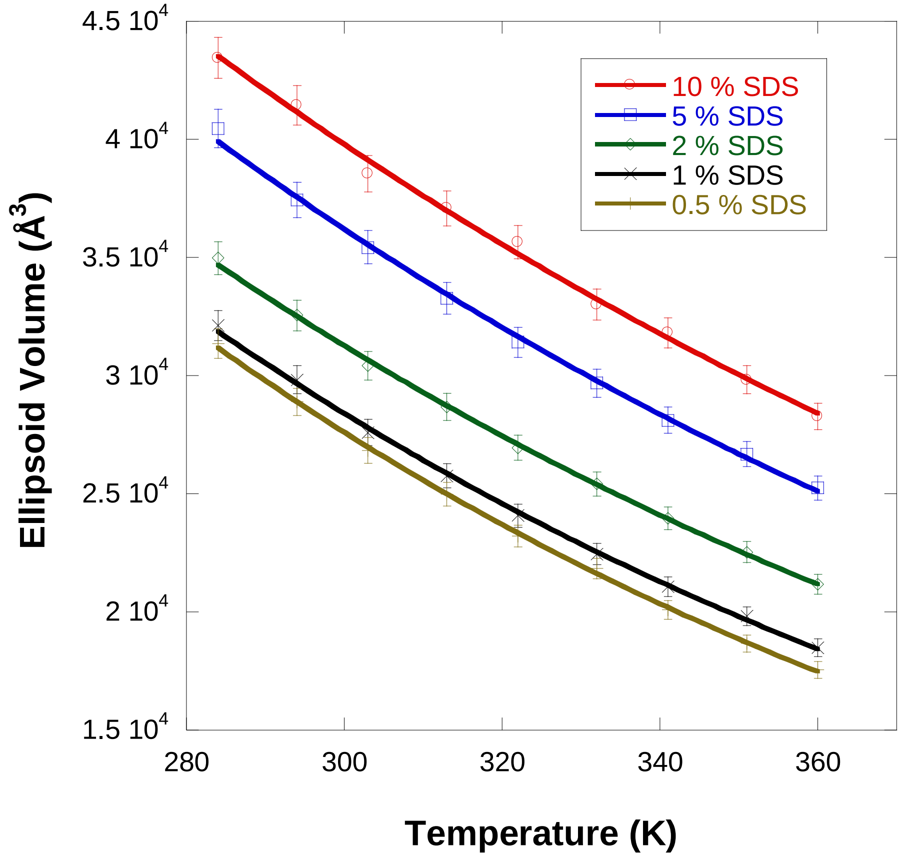


$$I(Q) = \frac{A}{Q^n} + \left[\frac{d\Sigma(Q)}{d\Omega}\right]_{\text{ellipsoids}} + B$$

$$\left[\frac{d\Sigma(Q)}{d\Omega}\right]_{\text{ellipsoids}} = \phi \Delta\rho^2 V_P P(Q) S_I(Q)$$

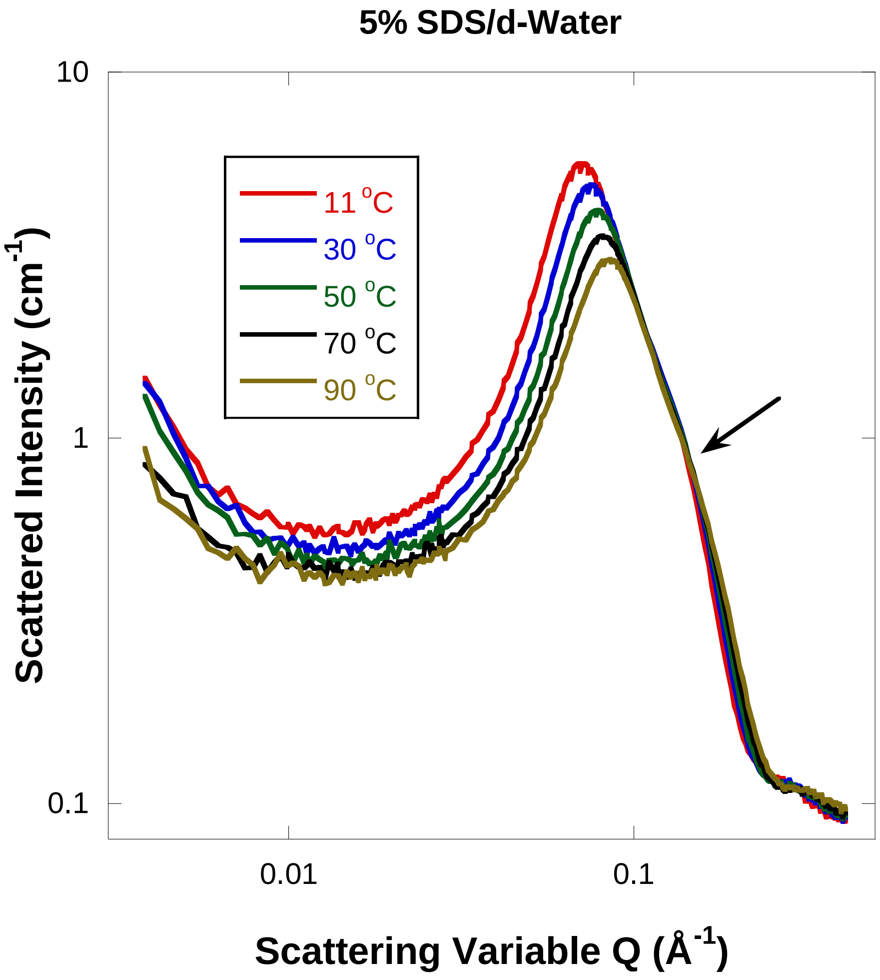
- Power law (low-Q) + ellipsoidal micelles (high-Q) model fits well

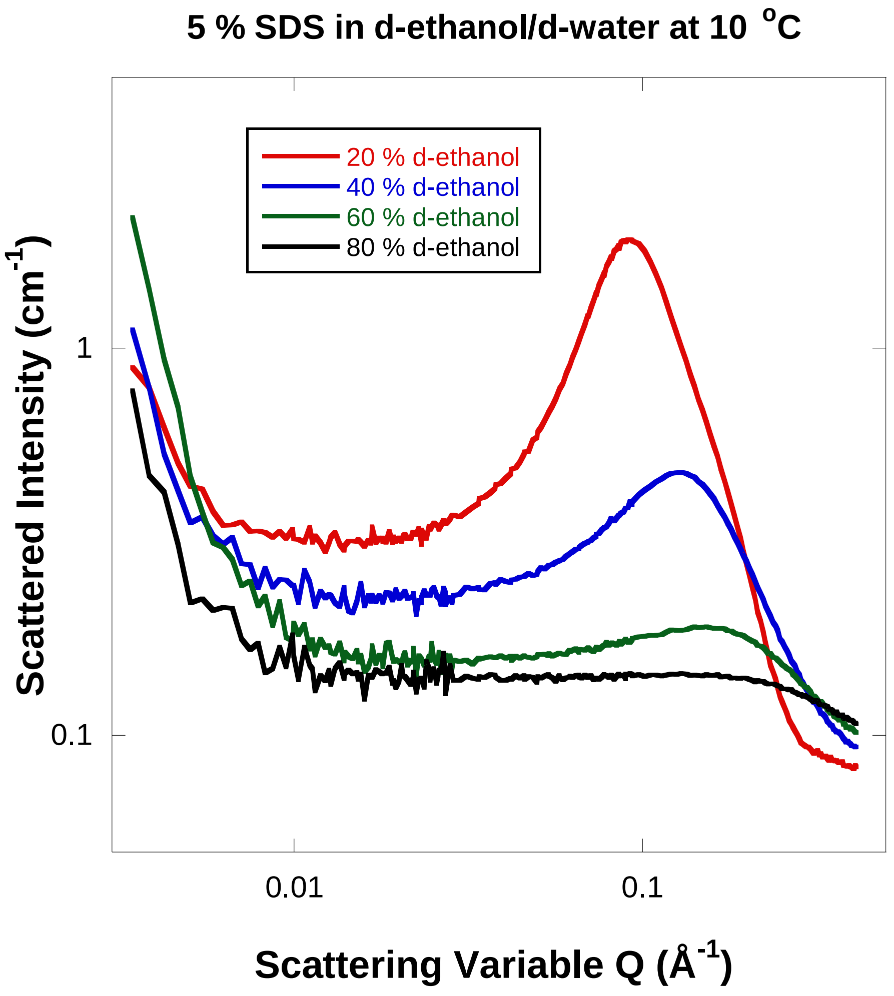
Some Fit Results



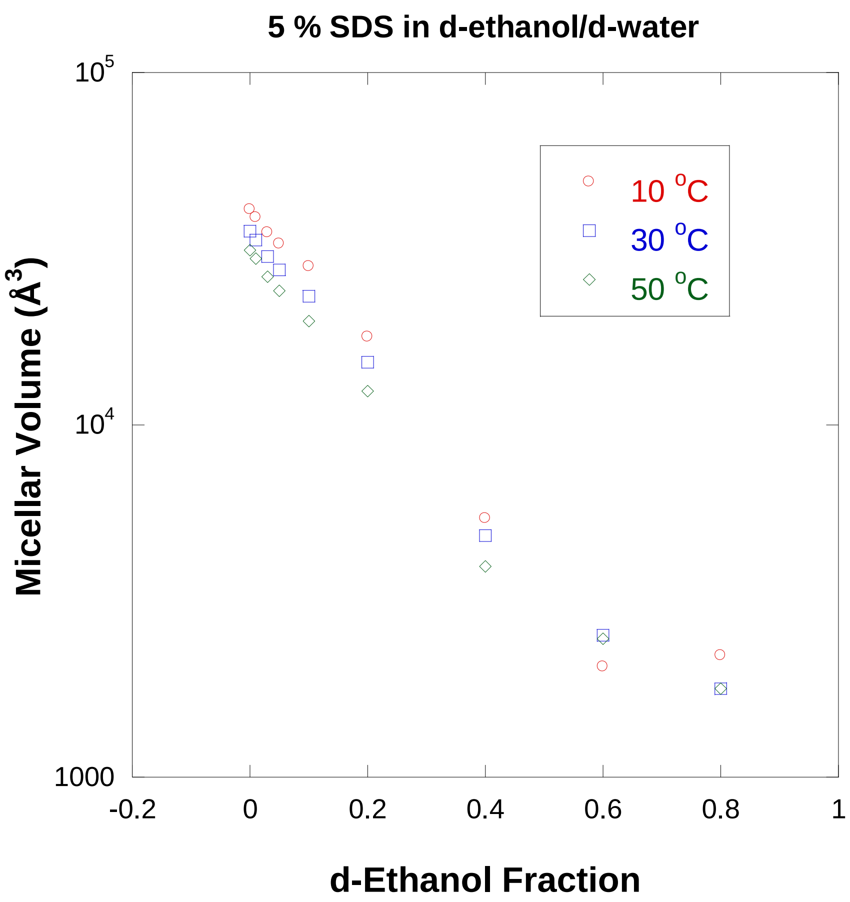
- Micelles become smaller at higher temperatures and lower volume fraction

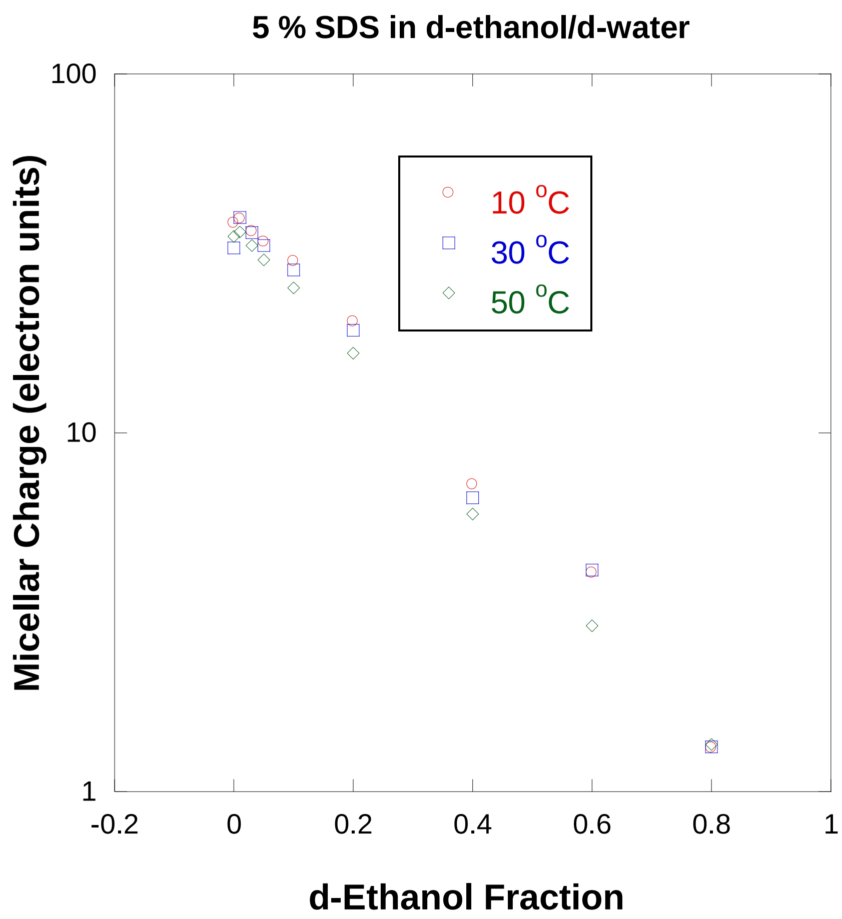
Varying Temperature and SDS Fraction



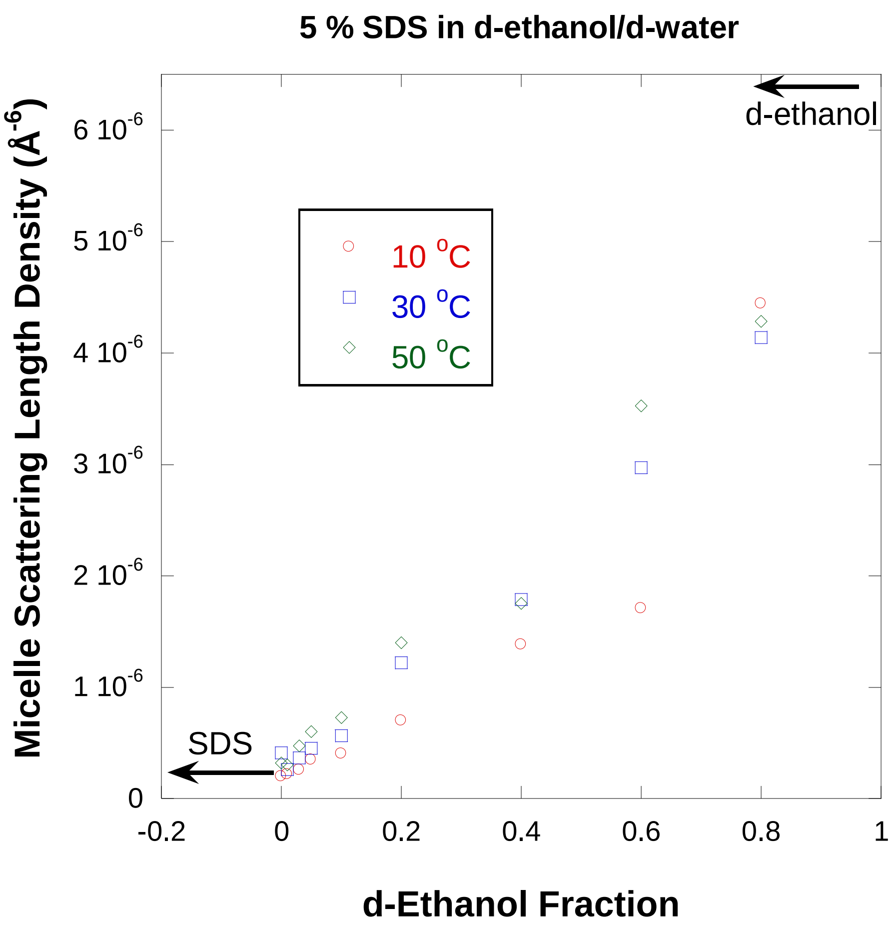


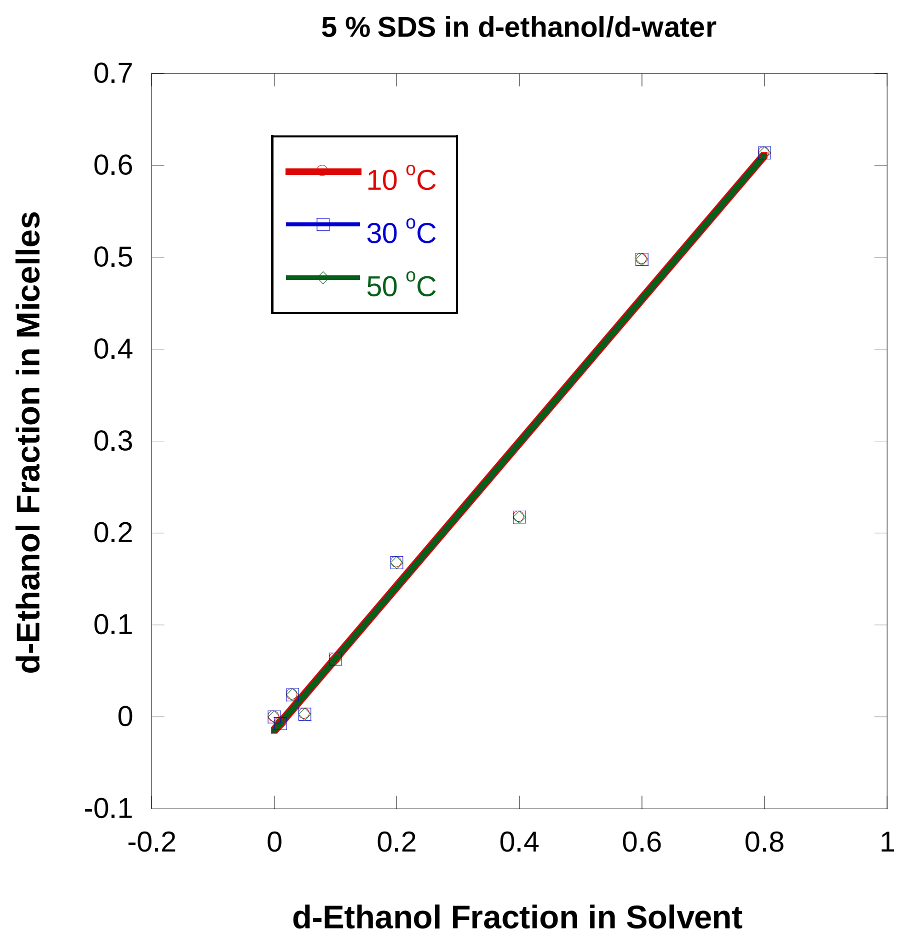
Adding Ethanol Co-surfactant





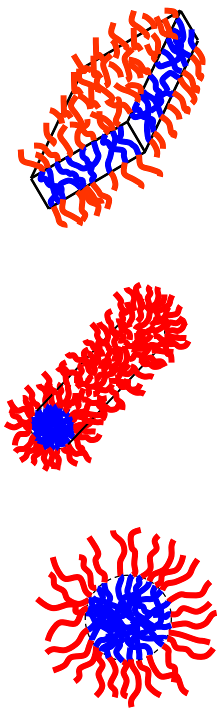
Adding Ethanol Co-surfactant



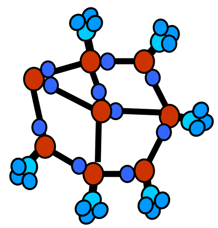


Summary –All Three Projects

P85 Micelles



PEO and PNIPAM Polymers

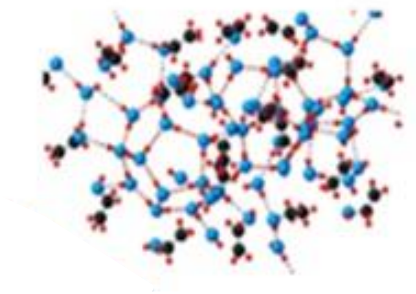


CH_3CH_2-OH H-OH

-CH_2CH_2-O- PEO

-CH_2CH_2-(O)NH-$(CH_3)_2$-
PNIPAM

SDS Ionic Micelles



Cage-like Structures