9/21/01 (#1)

H-Bonds 15-20 kJ/mol,
compared to ~400 kJ mol^{-1}
for covalent bonds.

But net strength is less because of water.
~5 kJ/mol but varies. Competition.
(≳1 kcal/mol)

Hydrophobic Interactions "(Bonds?)"
water fear

Propane C_3H_8 in water.

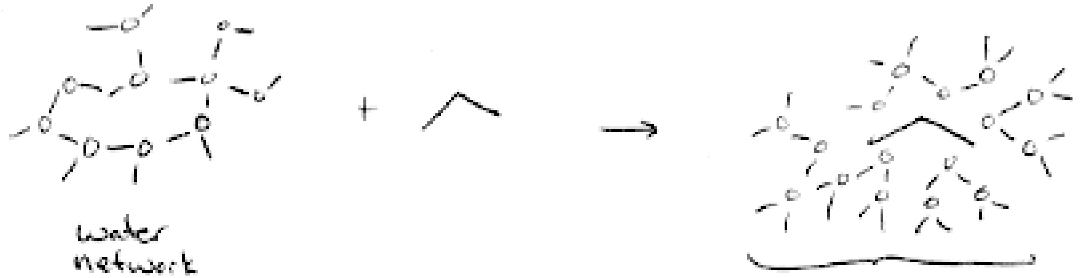
$$C_3H_8\ (l) + \infty H_2O \rightarrow C_3H_8\ (aq)$$

T = 298K
↓
$-T\Delta S = +24\ \text{kJ mol}^{-1}$

$$\Delta H^\circ_{298} = -8\ \text{kJ mol}^{-1}$$ favorable Huh?!

$$\Delta S^\circ_{298} = -80\ \text{J K}^{-1}\ \text{mol}^{-1}$$ unfavorable

$$\Delta G^\circ_{298} = +16\ \text{kJ mol}^{-1}$$ unfavorable NET.



Lots of H-bonds

Still lots of H-bonds, but fewer ways to do it.

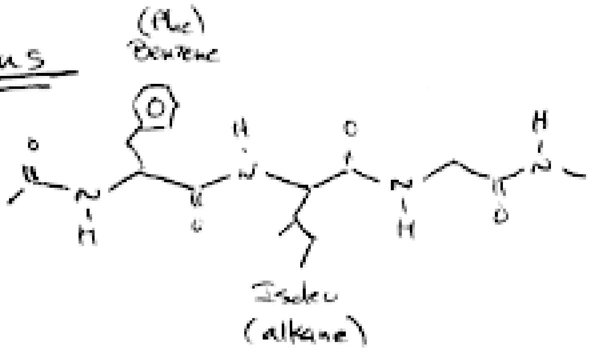
ORDER EXTENDS MANY/SEVERAL LAYERS OUT

The "bonding" here is the water.

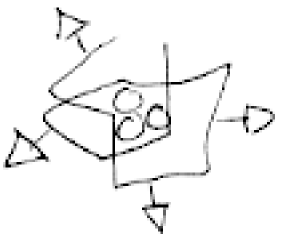
Entropy ⇒ This drives the phase separation of oils (propane is an alkane) in water

But not the ΔH of the water.
Rather, it's the ΔS of the water that drives phase separation.

Proteins

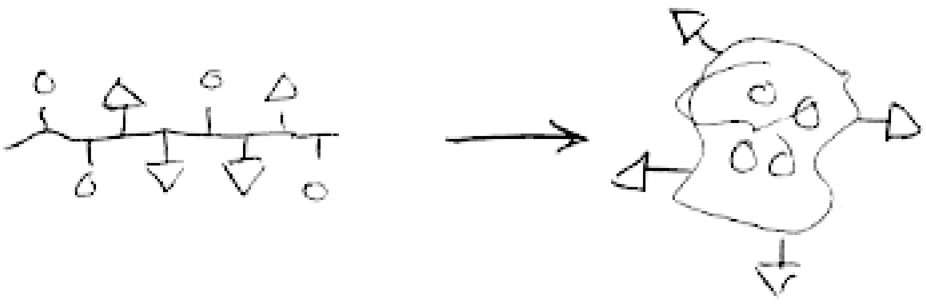


Amphiphilic
(Both)



O ≡ hydrophobic side chains

Δ = hydrophilic



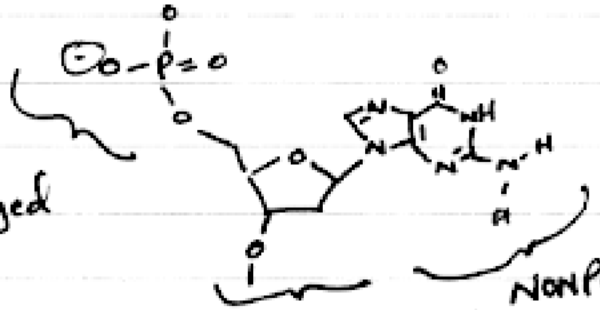
Protein-Folding
Equals
Taking Benzene
out of water!

Favorable. $\uparrow S_{H_2O}$

300
80
24000

Similarly DNA →

9/21/01

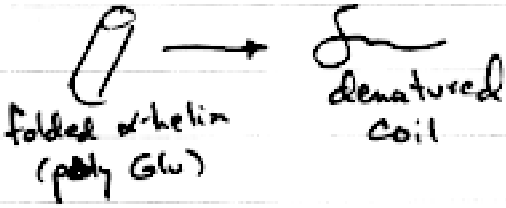


Stacking
van der Waals
London

Watson-Crick H-Bonds do NOT drive helix formation
Oil-water phase separation DOES
(+ ion solvation).

Recent exp'ts More hydrophobic base analogs with no H-bonding yield more stable double helices!

NUMBERS →

	ΔH°	ΔS°
 folded α-helix (poly Glu) → denatured coil	4.5 kJ/mole amide	
 lysozyme →	≈ 450 kJ/mole protein	
 DNA Duplex →	~ 35 kJ/mole bp ↙ ~30 AT ~44 GC BUT....	≈ 88 $\frac{J}{K\ mol\ bp}$ $T\Delta S$ ≈ 26 kJ/mol bp

88
300
26400

Review - Summary

MONDAY - WRITE ON A PIECE OF PAPER, PROBLEMS YOU'RE HAVING TROUBLE WITH

ΔG = Capacity to do work beyond PV

⇒ leads to spontaneity (driving force)

$\Delta G < 0$ spontaneous $\Delta G = 0$ Equilib $\Delta G > 0$ reverse

---

2^{ND} LAW → Entropy of the universe increases.

$$\Delta G_{sys} + \Delta S_{surround} \geq 0$$

$$\Delta G_{\text{phase change at equilib}} = 0$$

Use these to understand the energetics of changing T (or P)

$$q = \Delta H = n\bar{C}_p(\Delta T)$$

$$\Delta S = n\bar{C} \ln T_2/T_1$$

$\bar{C}_p$ or $\bar{C}_v$ for solids and liquids, they're about the same

Membranes Complex solutions

Phases are more complicated than liquid and solid.

Use this to understand a phase change at constant T and P

$$\Delta G^{\text{phase change}}_{\text{equil}} = 0$$

ie. at boiling/melting point

$$\therefore \Delta S^{\text{phase change}} = \frac{\Delta H^{\text{phase change}}}{T}$$

at equilib

Chemical Reactions

$$\Delta S(T_2) = \Delta S(T_1) + \int_{T_1}^{T_2} \Delta C_p \frac{dT}{T}$$

$$\Delta G(T_2) = \Delta G(T_1) - (T_2 - T_1)\Delta S$$

<u>IF</u> ΔS
is indep
of T
(ie. $\Delta C_p = 0$)