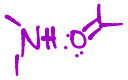
- MOTIVATIONAL TALE
- GOALS
- $\Delta G$ REVIEW QUIZ
- ROAD MAP

BRAINSTORM ATOMS
CALCULATE $\Delta G$

CHNOPS

| TYPE | NATURE | ATOMS | ~$\Delta G$ | RATIO FORMED/BROKEN |
|---|---|---|---|---|
| COVALENT |  | CHNOPS | 400 | $6 \times 10^{69}$ |
| IONIC |  | HNOP | 70 | $2 \times 10^{12}$ |
| H-BOND |  | HNO (S) | 20 | $3 \times 10^{3}$ |
| VDW |  | CHNOPS | 1 | 1.5 |

KEY
SCREEN
ME
STUDENTS
BOARD

CONTEXT:
- GEOMETRY
- WATER!

- $\Delta G$ FROM EQN
- PUZZLE

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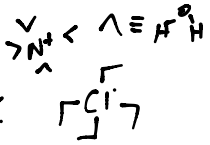
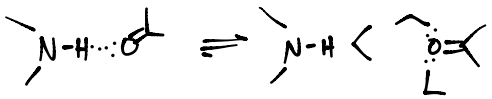
BUT WHAT ABOUT WITH WATER?

$$K = \frac{[Na^+][Cl^-]}{[NaCl]} \rightsquigarrow -RT\ln(K) = \Delta G$$

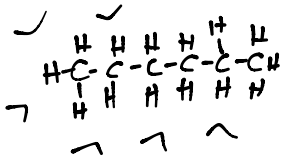


$\Delta G \ll 0$.

WHAT ABOUT H-BOND?



WHAT INTERACTIONS CAN HEXANE FORM?

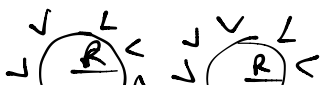


SHOW HAPPY WATER VISUAL.

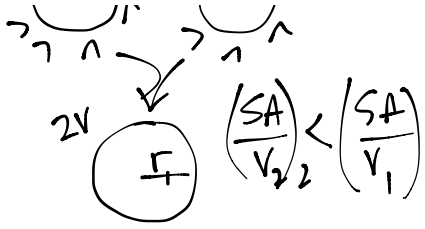
WATER FORMS UNHAPPY SHELL..

$\Delta G = \Delta H - T\Delta S$ $\quad \Delta S < 0 \rightarrow \Delta G \uparrow$

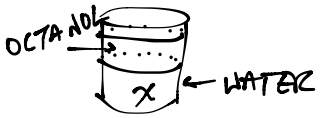
SO WHO CARES?



HYDROPHOBIC EFFECT

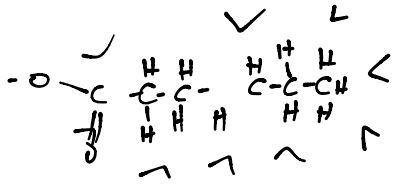



HOW "STRONG" IS HYDROPHOBIC EFFECT? // WOULD WE MEASURE?




$\Delta G_{H2O \to OCT} = -RT \ln \left(\frac{[X]_{OCT}}{[X]_{H2O}}\right)$

MOST HPHOBE AA : -13.6 kJ/mol
HPHIL AA : 10.4 kJ/mol



SATIS- ING CONFLICTING CONSTRAINTS

~ORDER

START WITH INSPIRATIONAL TALE → SELF ASSEMBLY ACROSS SCALES.

# LECTURE 2

TODAY COVER BUILDING BLOCKS → THE PARTS LIST.

## BIG THEMES.

- STRUCTURE → FUNCTION
- MASSIVE DIVERSITY VIA COMBINATORICS

## BY THE END OF LECTURE, YOU SHOULD

- UNDERSTAND THE BASIC MOLEC INTERACTIONS THEY FORM
- LOOK @ STRUCTURE AND/ PREDICT PROPERTIES

## FOUR MAJOR MOLECULES

PROTEINS
NUCLEIC ACIDS
LIPIDS
SUGARS
(LOTS O' SMALL MOLEC...)

SHOW STRUCTURES ON SCREEN

WHAT DO THESE MOLEC HAVE IN COMMON?

ATOMIC MAKE UP

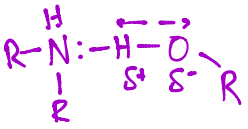
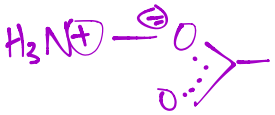
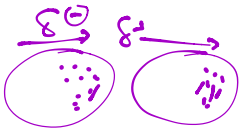
ONLY SIX ATOMS, ARRANGED DIFFERENT WAYS GIVE BIO DIVERSITY.

WHAT MAKES THESE DISTINCT?

SUGAR: HYDROXLS; FOOD/LUBRICANT

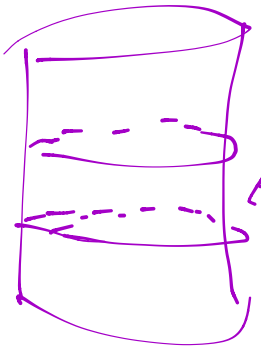
ETC.

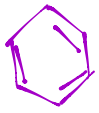
WALK THROUGH INTERACTIONS THESE ATOMS CAN FORM

| TYPE | NATURE | $\Delta G_{FORM}$ |
|---|---|---|
| COVALENT |  | $\cong$ -350 kJ/mol |
| HYDROGEN BOND |  | ~ -15 kJ/mol |
| ELECTROSTATICS |  | ~ -15 kJ/mol |
| VAN DER WAALS |  | ~ -5 kJ/mol |

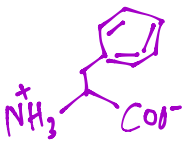
VARIES WITH DIST? ANGLE

NON: HYDROPHOBIC EFFECT





HEXANE

$Na^+$
WATER



PHE ?

MIX SOLUTION AND ASK HOW MUCH IN EACH PHASE. HOW DO YOU DESCRIBE SUCH A THING?

$$K = \frac{HEXANE}{WATER} = \frac{6.993\ M}{0.007\ M} = 141.9$$

$$-RT\ln(K) = -0.0083 \times 300 \times \ln(141.9) = -12.3\ kJ/mol$$

LYS +23.2

ON SCREEN, SHOW MD SIM OF PHE. (FRAME 20381)

START W/ PHE
SHOW WATER AROUND $NH_3^+$ AND $COO^-$; DISCUSS
SHOW WATER AROUND BENZENE

KEY PROPERTY: AMPHIPATHY
BOTH + SUFFERING

BROADEST DIVISION:
WATER-LIKE
OIL-LIKE

SIMPLE CALC: ENERGY TO MOVE ION PAIR TO INTERIOR