Week 2

Families of Carbon Compounds / Acids and Bases

2.1 Families of Carbon Compounds

10/7:

- Hydrocarbons:

  - Alkanes (C_nH_{2n+2}) and cycloalkanes C_nH_{2n}.
  - Alkenes (C_nH_{2n}).
  - Alkynes (C_nH_{2n-2}).

- Aromatic:

  - Contains a benzene ring.
  - All bonds $\sim 140\,\text{Å}$.
  - All carbons sp^2.
  - Planar.
  - π electrons above and below the ring.
  - Special stabilization.

- Covers drawing dipoles.

- Polar and nonpolar molecules:

  - Dipole = distance × change between charges.
  - $\mu = r \times Q$
  - $1\,\text{D} = 3.336 \times 10^{-30}\,\text{C m}$.
  - Analyzes molecules by drawing a Lewis structure, drawing a dipole along each bond, and drawing and labeling a net dipole, if applicable.
  - Goes through a number of examples.
  - Acetonitrile is a strong polar solvent.

- **Functional group**: A common arrangement that determines shape, bonding physical and reactivity of organic compounds.

- Families of carbon compounds:

  - Hydrocarbons: Aliphatic, aromatic.
  - Methyl, ethyl, propyl, R = alkyl groups.

- Phenyl: Ph- or ϕ-.
- Benzyl: $Ph-CH_2$-, $C_6H_5CH_2$-, Bn-
- Compounds with R$-$Z where Z is a heteroatom.
  - ■ If Z is a halogen X, then the halogroup makes it an alkyl halide or haloalkane.
- Alkenyl halide: $X-=$.
- Aryl halide: Ph$-$X.
- Alcohols or phenols: R$-$OH.
- Ether: R$-$O$-$R′.
- Amines: NH_2R, NHRR′, NRR′R″.
- Thiols or mercathols: R$-$SH.
- Carbonyl group: R$-$CO$-$R′.
- Aldehyde: R$-$COH.
- Ketone: R$-$CO$-$R′.
- Carboxylic acid derivatives:
  - ■ Acid: R$-$COOH.
  - ■ Ester: R$-$COOR′.
  - ■ Acid chloride: R$-$COCl.
  - ■ Acid halide: R$-$COX.
  - ■ Amide: $R-CONH_2$.
  - ■ Acid anhydride: R$-$COOCO$-$R′.
- Nitrile: R$-$C$\equiv$N.
- Acrylonitrile: $=-$C$\equiv$N.

2.2   Discussion Section

- ACS in-text citations should be in superscripts as a list of number with no brackets or parentheses.

- Molecular formulas are C_2H_6O, not C_2H_5OH or CH_3CH_2OH.

- Make a table if you have a lot of data to put in (make it readable!).

- Distillation:

  - We need a boiling chip and stir bar inside the flask.
  - Vapor comes up from a round-bottomed flask, encounters a rubber stopper and gets diverted through a condenser instead.
  - Make use of countercurrent exchange and increase pressure by inflowing water in the gravitationally lower portion of the condenser.
  - Boiling chip is a coarse material with a lof of micropores inside.
  - The surface energy is reduced when the fluid is inside the micropores; within, it can more easily become a gas.

- As the mole fraction χ of a substance A increases...

- Raoult's law:
$$P_{\text{total}} = \frac{P_A\chi_A}{P_B\chi_B} = \frac{P_A\chi_A}{P_B(1-\chi_A)}$$

- Dalton's law: The total pressure is equal to the sum of the partial pressures.

2.3 Intermolecular Forces and IR Spectroscopy

10/12:
- Intermolecular forces and physical properties.

- **Boiling point**: The temperature at which the vapor pressure is equal to the pressure of the atmosphere above.

  - The stronger the intermolecular forces, the higher the boiling point.
  - The higher the molecular weight, the higher the boiling point.

- **Melting point**: The temperature at which the crystalline solid and liquid are in equilibrium.

  - The stronger the intermolecular forces, the higher the melting point.
  - The more symmetrical, the higher the melting point.

- Solubility.

- Intermolecular forces.

  - All electrostatic attractions related to bond polarity.
  - 3 types: Dipole-dipole forces, hydrogen bonding, and dispersion forces.

- **Dipoloe-dipole forces**: Attraction between opposite poles ($1 \, \text{kcal/mol}$ to $3 \, \text{kcal/mol}$).

- **Hydrogen bonding**: Dipole-dipole interaction between H-atoms bonded to O, N, F ($2 \, \text{kcal/mol}$ to $10 \, \text{kcal/mol}$).

- **Dispersion forces**: Weak ($< 1 \, \text{kcal/mol}$). Momentary distortion of the electron cloud (temporary dipole). Induces dipoles in surrounding molecules. *Also known as* **London forces**.

  - Depends on **relative polarizability**.
  - Dependes on the surface area of the molecule — more surface area means more distance electrons can spread apart.

- **Relative polarizability**: How far valence electrons are from the nucleus.

- Solubility:

  - For something to be soluble, you need to have favorable forces between them.
  - Ionic compounds are soluble in water, less soluble in polar solvents, and insoluble in nonpolar solvents.
  - Organic compounds: < 3 carbons is soluble, 4-5 carbons is borderline, ≥ 6 is insoluble. More soluble in organic solvents.

- Organic solvents:

  - CH_2Cl_2 — methylene chloride.
  - $HCCl_3$ — chloroform.
  - H_3CCOCH_3 — acetone.
  - Diethyl ether.
  - THF.
  - Cyclohexane.

- In TLC, the silica gel is very polar, so polar compounds will not move far up the plate. Nonpolar solvents will drag nonpolar compounds up pretty high.

- HOMO and LUMO get closer as conjugation increases.

- IR spectroscopy:

– The frequencies absorbed vary based on the type. Higher stretching frequencies for lighter atoms and stronger bonds.

– IR radiation causes transitions in vibrational modes of bonds.

– The stronger the bond and the lighter the atoms, the faster the vibration of the molecule and the higher the stretching frequency.

– The ΔE's are inherent characteristics of the bonds and nuclei.

– Bonds absorb light of characteristic energy, frequency, and wavelength.

– We usually report IR spectra in terms of the wavenumber $\bar{\nu}$.

– The frequencies absorbed can indicate bond types and functional groups in the molecule.

– Anything above 1500 (of wavenumber less than 1500) is called the **fingerprint region** — it may not tell you what a molecule is, but it will tell you if two molecules are the same.

– Sharp peaks at high wavenumbers are characteristic of $N-H$ interactions.

– Make a line at $3000\,\mathrm{cm}^{-1}$. Things to the right of that indicate aliphatic $C-H$'s. Things to the left indicate sp^2 $C-H$ groups. Things more to the left indicate sp $C-H$ groups.

– Not all bonds are visible — stretching bands must change the dipole. Thus, for example, the $C{=}H$ stretch in trans-but-2-ene is not IR active, but the $C{=}H$ stretch in cis-but-2-ene is IR active.

– If you want to substitute D for H, the peak formerly associated with the $R-H$ bond will move lower.

COMMON ABSORPTIONS	
Aromatic $C-C$	Two peaks usually in the range of $1500\,\mathrm{cm}^{-1}$ to $1600\,\mathrm{cm}^{-1}$
$C{=}C$	$\sim 1650\,\mathrm{cm}^{-1}$
$C{=}O$	$\sim 1710\,\mathrm{cm}^{-1}$ (shifts to $\sim 1735\,\mathrm{cm}^{-1}$ for esters)
$C{=}C$	$2100\,\mathrm{cm}^{-1}$ to $2300\,\mathrm{cm}^{-1}$
$C{=}N$	$2100\,\mathrm{cm}^{-1}$ to $2300\,\mathrm{cm}^{-1}$
$C-H$ (aldehyde)	Two peaks at $2170\,\mathrm{cm}^{-1}$ and $2810\,\mathrm{cm}^{-1}$
sp^3 $C-H$	Just to the right of $3000\,\mathrm{cm}^{-1}$
sp^2 $C-H$	Just to the left of $3000\,\mathrm{cm}^{-1}$
sp $C-H$	$\sim 3300\,\mathrm{cm}^{-1}$
$N-H$	$\sim 3300\,\mathrm{cm}^{-1}$ (one peak for $-NH-$, two peaks for $-NH_2$)
$O-H$ (alcohol)	$\sim 3400\,\mathrm{cm}^{-1}$ (a broad, smooth peak)
$O-H$ (acid)	$\sim 2500\,\mathrm{cm}^{-1}$ to $3500\,\mathrm{cm}^{-1}$ (a very broad, ugly [not smooth] peak)

Table 2.1: Common IR spectroscopy absorptions.