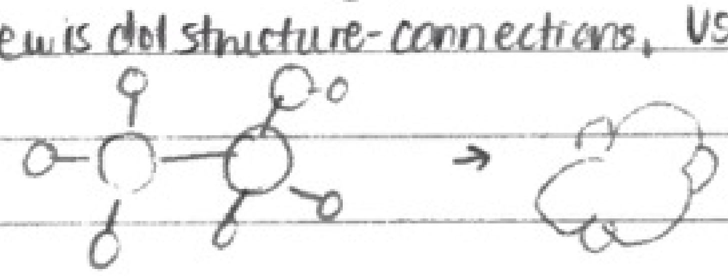
10/24/13 Why is everything so different?

- Today we will
    - use VSEPR, VB, and MO to get a better picture of POLAR and NONPOLAR molecules
    - recognize different molecules have different physical properties
    - classify intermolecular forces
- VB - local "bonds"
  MO - delocalized - whole molecules
- Combine VB and MO theory

 carbons have sp^2 hybridization

π bonds - use MO theory
σ bond - use VB theory →

- resonance structure - the double bond is spread throughout the molecule. Pi electrons are everywhere and so they are delocalized
    - ↳ Delocalized electrons associated w/ resonance.
- Visualize ethanol
    - we use VSEPR and VB to get visual image
    - we predict polarity just from the ball and stick model
    - Lewis dot structure - connections, VSEPR shape



- chemical composition and shape
    - C_2H_6 gas (ethane)
        - ↳ add OH: Ethanol - liquid at RT
    - $C_{24}H_{50}$ (oil) liquid at RT. so there must be some interaction between the molecules
    - What is the density of a liquid?
        - ↳ Gas density, we use MW, but this is not the case for liquid. Liquids depend on how well you can pack electrons together.
- Physical properties
    - What dominates the interaction in condensed phases?
        - ↳ What are these forces? How are they classified.
        - ↳ Define Intermolecular forces (IMF) these are electrostatic forces
- Identify a few trends. (trends hold for similar compounds)
    1. As molecular weight increases, then it seems that BP increases (sort of)

2. Long molecules have some sort of higher boiling point.

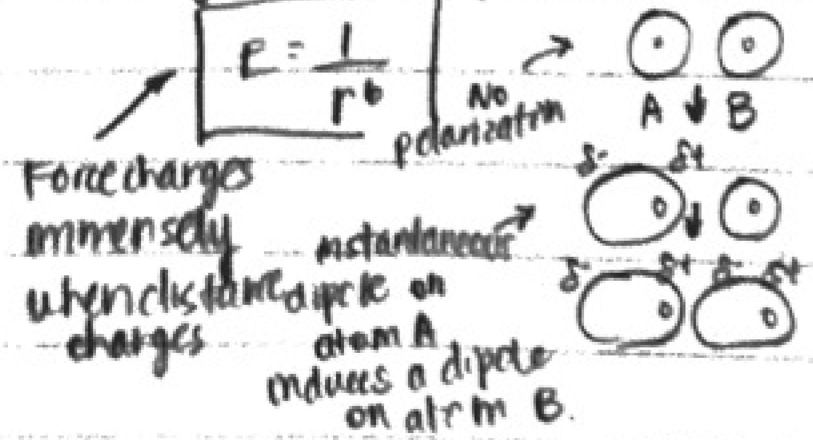
3. Polar molecules have high BP (sort of true)

4. The more OH "groups" (you can associate OH as a polar group/region), the higher the temperature.

- Intermolecular Forces
  - The dominate force in chemistry is coulombic
  - The boiling point of NaCl is 1413°C. Why is it so high? STRONG FORCES
  - Qualify the word "intermolecular" - between molecules, "particles"
  - The molecule is in a condensed phase, but not ionic
    - ↳ A molecular condensed phase is a molecular liquid or molecular solid.
    - ↳ "Particle" is a molecule
    - ↳ Lower E when molecules are close.
- IMF: Dipole-Dipole
  - attractive force between partial - end of one molecule and partial + end of another molecule.
  - Strength depends on DISTANCE and dipole moment

    $E = \frac{1}{r^3}$ "polar" $\mu \neq 0$

    Depends on magnitude of μ (dipole)
    - ↳ If you move molecule far apart, this force will disappear
- All nonpolar compounds are NOT gases
  - ↳ if BP > than room temperature, then the substance is a liquid.
  - ↳ when molecular weight goes up, it seems forces are getting stronger.
- IMF: Fact Check
  - How is it possible for hexane and CCl_4 be liquids? Must be electrostatic force.
- IMF: Induced dipole Induced dipole
  - Exist in ALL condensed substances
  - Caused by induced dipoles, which come and go in nonpolar molecules and atoms.



* Polarizability - how do electrons "react" to a nearby charge. This is related to how tightly electrons are held.

  - Names: Induced-Dipole Induced-Dipole, Dispersion forces, London Forces, Van der Waals forces. These are the same.

- consider an array of atoms and molecules

Helium	4	-268.9
Krypton	83	-153.2
Propane	44	-42.1
CCl_4	154	77
octane	114	126
	↑ MW	↑ BP

- The IMF strength is dependent on shape and polarizability because MW sometimes tells you about shape and polarizability.

 Propane

 octane. Shape is now longer.

Polarizability
- Induced-Dipole induced dipole forces exist in ALL condensed substances
- Strength depends on POLARIZABILITY
- move down periodic table, the polarizability increases
    - ↳ this occurs bc there are more electrons, and the electrons are farther from nucleus.
- Halogens: F_2 (gas) Cl_2 (gas), Br_2 (liquid), I_2 (solid)

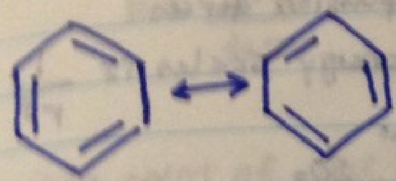
- SHAPE
    - Why can't the charged glass rod induce a dipole?
        - Distance Dependence is HUGE bc the rod is never close enough
    - This is why shape is so important - how close can the individual atoms get to each other in space?
    - FAVORITE Analogy: VELCRO - interactions all the way along molecule. As a result, it is not a point interaction, but an interaction throughout the molecule

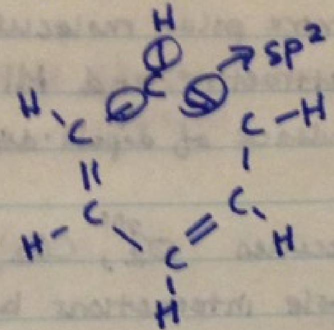
- We can evaluate SIMILAR Molecules
    - The BP of Sn hydride is less than the BP of the Te hydride bc the Sn compound has a smaller dipole. (SnH_4 vs. H_2Te) Lower BP = less interactions
        - ↳ polarizability about the same bc they are in the same row.
        - ↳ smaller dipole, so less interactions
    - The BP of S hydride is less than the BP of the Te hydride because the S compound is less polarizable
        - ↳ bc sulfur is higher on the periodic table so more polarizability
    - The BP does not seem to follow the trend for which period? 2

- IMF: Dipole-dipole
    - Hydrogen bonding - special type of Dipole-Dipole Force - particularly strong bond
    - Occurs w/ N, O, F
    - Stuff w/ OH will usually have hydrogen bonds

Combine MO and VB Theory

C_6H_6 Benzene





trig planar!

use MO to describe resonance

↳ delocalized picture of π ~~bond~~ orbital → rep by 

[LM 23] ~~///~~ **Forces of Attraction**

Types of Interactions

- forces driven by electrostatics, forces felt betw charged particles

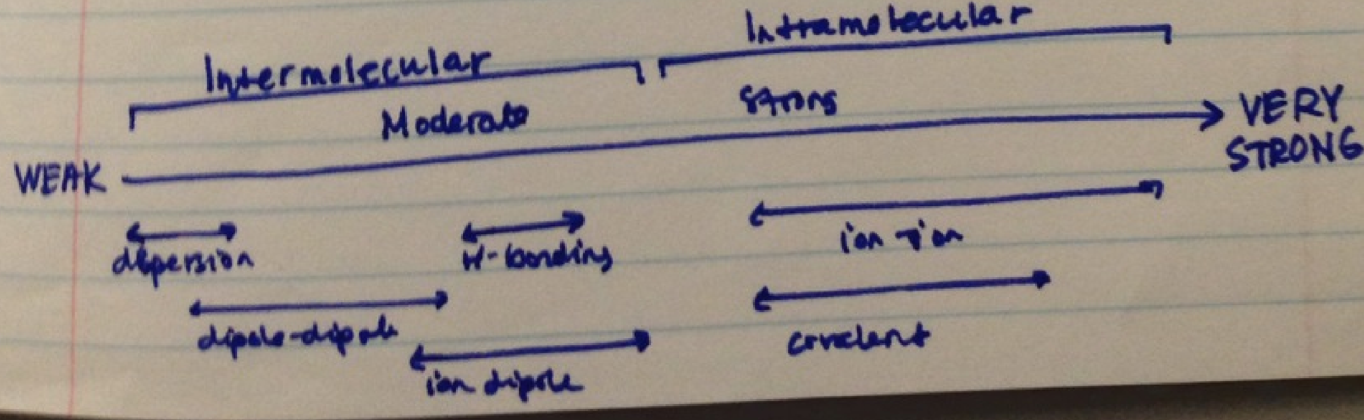
dipole-dipole forces – forces between polar molecules (mol. w/ permanent μ)

hydrogen bonding – extreme dipole-dipole forces, occurs when Hydrogen atom bonded to a HIGHLY electronegative atom (MUST be O, N, or F)

dispersion forces – "weakest" but most important since ubiquitous → EVERY molecule has dispersion forces (London, vander waals, induced-dipole)

- degree to which a molecule has D.F. is measured by polarizability Polarizability (α) : non-polar :: μ : polar $E = \frac{1}{r^6}$

temporary dipole moments!!



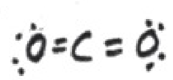
$E \propto \frac{1}{r^3}$ (molecules **must** be polar!)

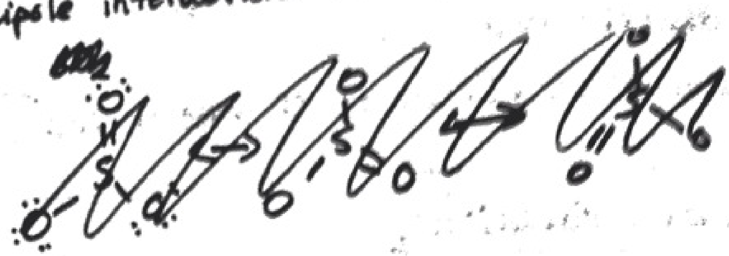
Dipole-Dipole

- when two or more polar molecules come together, try to MAX attractive and MIN repulsion forces
- distance dependence of dipole-dipole energy scales is $\frac{1}{r^3}$

Q: For which molecules O_2 (no), CO_2, O_3 (no), SO_2 will dipole-dipole interactions be important???

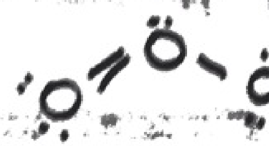
CO_2





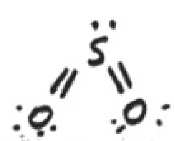
O_2

O_3 POLAR!



SO_2

N A
24 18
$\frac{6}{2} = 3$ bonds



THURS LECTURE

Dominant Force in Chem is Coulombic

$$E = \frac{q_1 q_2}{4\pi\epsilon_0 r} \qquad E \propto \frac{\text{charge}}{\text{distance}} \qquad E \propto \frac{1}{r}$$

- boiling point of NaCl is 1413°C. Why is it so high?