CHAPTER 2

ORGANIC COMPOUNDS: A FIRST LOOK

2.1 Common bonding situations

- Direction
  - Satisfying the octet rule
  - Lowering the formal charge
- Hydrogen
  - Always single bond
- Carbon
  - Stable – neutral – single, double, or triple
  - Unstable – carbanion, carbocation, radical

- Nitrogen
  - Stable – neutral – single, double, or triple
    - With a lone pair e^- (unshared pair of e^-)
  - Charged N is also relatively stable

- **Oxygen**
  - **Stable – neutral – single or double**
    - **With two unshared pairs of e$^-$**
  - **Charged O is also relatively stable**

- **Halogen**
  - Stable – neutral – single
    - With three lone pair e^-
  - Charged (-) halogen is stable

- **Phosphorous**
  - Similar to N

    >8 outer shell e^-

- **Sulfur**
  - Similar to O

    >8 outer shell e^-

2.2 Bond strength and bond length

- **Bond Strength ◄ Bond dissociation energy**

  - **Energy for homolytic cleavage at gas phase**
  - **Structure-dependent**

    CH_3-H (104 kcal/mole), C_2H_5-H (98), $(CH_3)_3$C-H (91)

- **Trends (*see Table 2.1-2.2, next page*)**
  - **The stronger, the shorter Y-H strong (~100 Kcal/mol, 1 Å)**
  - **C-C stronger than C-Y or Y-Y’**
  - **Y-C relatively strong (70~80 Kcal/mol, 1.5 Å)**

    O-O and N-O (~35 Kcal/mol): due to repulsion between unpaired electrons
  - **C-X become weaker from F to I**
  - **single < double < triple**
  - **C-C bond is stronger and shorter that Si-Si (life based on Si ?)**

2.3 Constitutional (Structural) isomers (구조 이성질체)

Two or more compounds with

1. the same molecular formula (composition)
2. the different structural formula (connectivity)

CH_3CH_2OH and CH_3OCH_3 from C_2H_6O

of possible isomers ↑ as # of atoms ↑

A general method to calculate the number of isomers for a given molecular formula has not been developed.

Because it is too complex!

You need practice!

- **Practice**

  C_6H_{14}

Practice problem 2.1

So there are eight constitutional isomers that have the formular $C_5H_{11}Cl$

Line bond formula

- Draw the structural formula by
    - Drawing a line for a bond
    - Not showing C and H bonded to C

Three of many constitutional isomers

2.4 Degree of Unsaturation

Saturated hydrocarbon: C_nH_{2n+2}

Hydrocarbon with one double or saturated cyclic compound: C_nH_{2n}

Calculation the degree of unsaturation

Calculate the

DU = (max # H - # H)/2

ex) for C_nH_x, DU = [(2n + 2) - x] / 2

- # double bond and ring
- 1 triple bond = 2 double bonds

Halogen is counted as H, #H + 1

ex) $C_5H_{11}Cl = C_5H_{12}$

O is not counted

ex) $C_6H_{10}O = C_6H_{10}$

N has three bonding

therefore the max. # (+ 1) of H for $C_{10}H_{15}N$ is

$2n + 2 + 1 = 23$

Drawing structural isomers

STEP1: Calculate the degree of unsaturation

STEP2: Draw skeletal chain/structure from longer to shorter

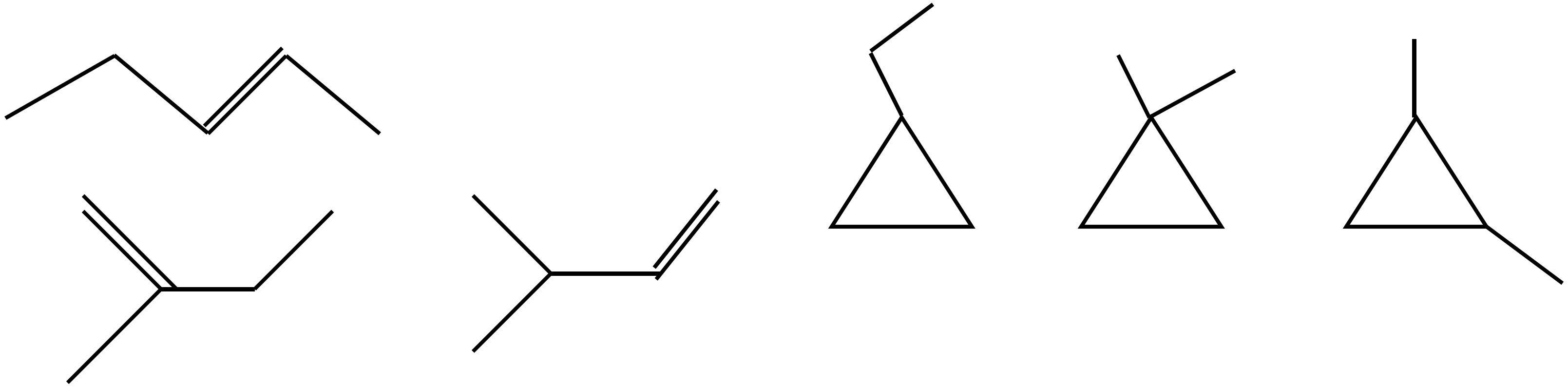
STEP3: Place heteroatoms

Practice, drill, and exercise

- **📖38-43 Problems 2.3 – 2.10**

Drawing 10 structural isomers of C_5H_{10}

Others



2.5 Structure & Property

Types of Intermolecular interaction

- **Charge-charge interaction, $(q_1 \cdot q_2) / r^x$**

1. ion-ion, ~200 kcal/mol (NaCl, 188 kcal/mol)

  - **covalent ~100 kcal/mol**

2. ion-dipole

3. dipole-dipole

4. dipole-induced dipole

5. instantaneous dipole-induced dipole
(London (dispersion) force)

3, 4, 5 - van der Waals forces (0.5 - 5 kcal/mol)

6. hydrogen bonding

dipole-dipole attraction between H on an electronegative atom (O, N, F) and an electronegative atom (O, N, F)

- fairly strong (3 - 8 kcal/mol) - why?

2.7 Melting point

solid to liquid – mobility, intermolecular interaction

ionic solid vs covalent molecule

higher mp for the molecules with stronger interactions

molar mass (molecular weight, size)

larger molecule have higher mp

because larger London forces

ex) propane < pentane

symmetric, compact (shape) molecules

Because pack into crystal lattice better

(close packing) ex) *n*-pentane < neo-pentane,
cubane > *n*-octane

Boiling point

- **Liquid to gas – separation**

- Trend is similar to mp
- Higher bp for

  stronger interactions

  larger molecules

  Symmetrical shape is not important (already moving around)

  high surface area rather than packing
  pentane > neo-pentane

- H-bonding is more influential than in mp
  - Butanol > ethyl methyl ether

Solubility

- $\Delta G_{mixing} = \Delta H_{mixing} - T\,\Delta S_{mixing}$
- For mixing 1 and 2 (dissolution 2 in 1) : $0 > \Delta G_{mixing}$
- ΔH is normally positive except there is a specific interaction (depends on interactions 1-1, 2-2 and 1-2)
- Δ S is normally positive because the more disordered state after mixing
- Rule of thumb ‘like dissolves like’
  - Hydrophilic vs Hydrophobic
  - Polar vs Nonpolar
  - Water-soluble vs Oil-soluble (organic)

Ex) NaCl is soluble in water, while pentane is not (consider ΔH & Δ S)

ethanol is totally soluble in water

butanol; 9g/100 mL, hexanol; 0.6g/ 100mL

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2.7 Functional groups

- **particular group of atoms where the reaction occurs = functional group**
- **Example: R-OH's (alcohols) show similar chemical reactions regardless of the types of R**
  - **ROH: R, alkyl group; OH, hydroxyl group determines way of reaction**
  - **Chemical reaction; attraction between positive and negative, or partial charges**
  - **C-O, O-H: reactive**
  - **C-C, C-H; not reactive**
- **determines physical property positive**

All ROH have very similar chemical behavior

functional groups