ORGANIC CHEMISTRY 1

Department of Chemical and Biological Engineering

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CHAPTER 1

A Simple Model for CHEMICAL BONDS

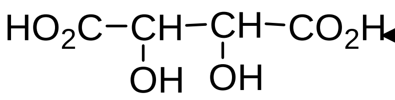
Contents: Organic Chemistry
Lewis Structure
Bonding
Shape of molecules

1.1 The Field of Organic Chemistry

What is Organic Compounds? sugar, alcohol, acetic acid !

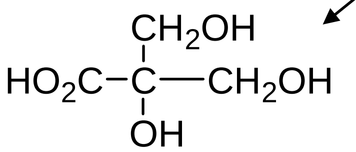
Why?

Carls Wilhelm Sheele's pioneering work in 1700s



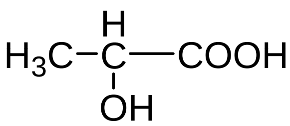
isolation of glycerol from animal fats

tartaric acid from grapes



citric acid from lemon or tangerines

lactic acid from sour milk



At that time nobody knows the chemical structures

Older Definition of these organic compounds

Compounds obtained from plants and animals

Inorganic compounds

Obtained from the minerals

These are quite reasonable because

organic compounds: low mp, low bp, low decomposition temp

Inorganic compounds: higher values

Antoine Lavoisier: The father of modern Chemistry

In 1774 he found that organic compounds burn to produce CO_2 and H_2O.

Therefore they are composed of **C, H, and O**. Later organic compounds from animal also contains **N.**

Before 1828,

Only a living organism can make an organic compound → 'Vital Force Theory'

In 1828 Wohler found that urea was formed when ammonium cyanate was heated.

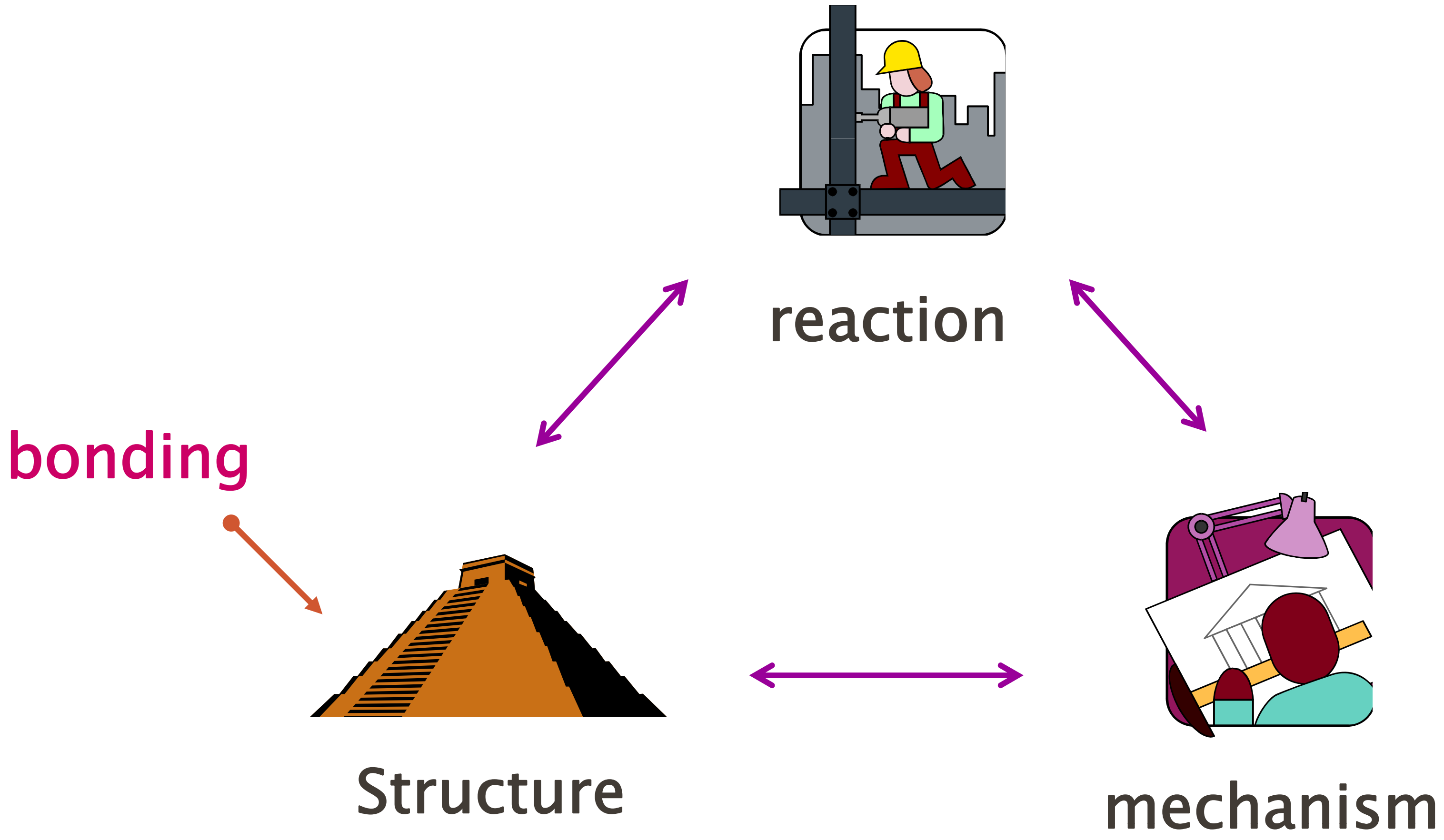
Urea: organic compound $H_2N\overset{O}{\overset{\|}{C}}NH_2$ from 소변

Ammonium cyanate: inorganic NH_4CNO

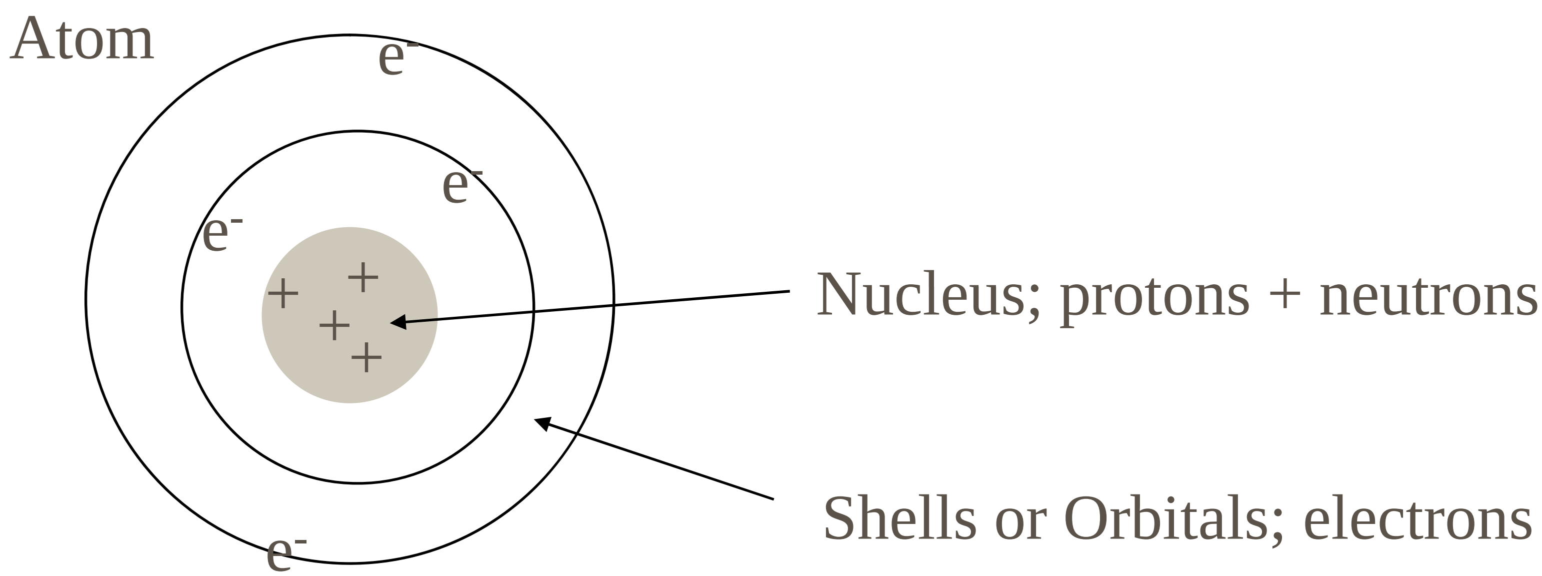
Therefore the definition of organic compound has been changed to

'The study of the compounds of carbon'

Components of Organic Chemistry



1.2 Simple Atomic Structure



Atom have an equal number of electrons and protons; neutral

The electrons in the outermost shell (valence electrons) control the chemical bonds

Nobel gases have a filled outer shell of electrons; very stable

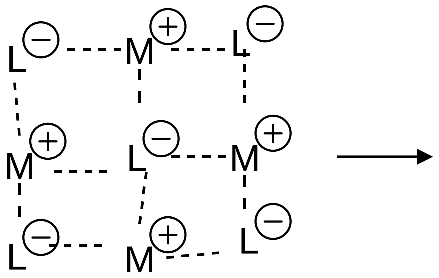
- Lewis structure

Lewis structure of some atoms

1.3 Ionic Bonding

The atoms gain or lose electrons to arrive at the same number of electrons as one of the nobel gas!

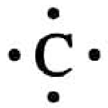
Then multiple intermolecular intxns are possible



High bp and mp

Ex) MgCl; mp=708 ^{o}C, bp=1412 ^{o}C

How about carbon.



$+ \ 4e^- = C^{4-}$

$- \ 4e^- = C^{4+}$

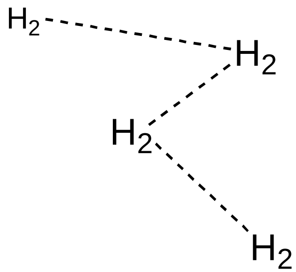
$\longrightarrow$ **Very difficult**

Therefore prefer to have covalent bonds

1.4 Covalent Bonding

The atoms share electrons to arrive at the same number of electrons as one of the nobel gas!

H• + H• ⟶ H:H or H-H or H_2



⟶ v.d.W intxn; very weak intxn

low bp and mp

mp= – 259 °C, bp= – 252 °C

- Other example

- Strong bonding between atoms -- molecule
- Weak intermolecular interaction -- low melting

1.5 Lewis Structures

How to represent Covalent Bonding

Too many dots; tedious

Therefore other shortened ways are commonly used

- Number of bonds **commonly** formed

H ; one covalent bond is possible

Atoms at second period need 8 atoms in their outer shell; **octet rule !**

If Octet rule is satisfied then the molecule is stable

Stability (←→Reactivity)

- 🕮 Problems 1.5 & 6
- CH_4 vs $\cdot CH_3$
- CH_3OH vs NH_5

How to Writing Lewis structure

- Satisfying the octet rule
- Bonding the atoms other than H first

Ex) CH_4O

Ex) C_2H_4

Ex) HCN

1.6 Covalent Ions

- Covalent compounds with charge (ion)

$$NH_3 + HCl \rightarrow NH_4^+ + Cl^-$$

neutral molecule	neutral molecule	covalent ion	ion

- calculation of charges:
  - Counting (# protons) - (# electrons)

    NH_4: 7 + 4 - 10 = +1, Cl: 17 - 18 = -1
  - Balancing the charges

    $0 + 0 \rightarrow (+1) + (-1)$

1.7 Formal Charges

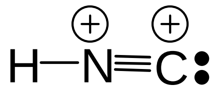
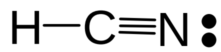
- Formal charge (FC)=

  (# valence e^-) – (# unshared e^-) – (# shared e^-)/2
- Σ FC of all atoms

  = total charge of the species
- Examples

HCN vs HNC

• Lewis structure	H:C:::N:	:C:::N:H
• Charge	0	0
• Formal charge	0 0 0	−1 +1 0
• Stability	>	

- Fewer formal charge → More stable
  -  vs 

- More complicated Lewis structure

Two oxygens are different according to the structure,

While they are the same according the experiments!

Why?

Resonance!

1.8 Resonance (공명)

- The actual structure of CH_3NO_2

- Any Lewis structure cannot represent the real molecule (experiment)
- the actual structure is a resonance hybrid

- resonance arrow ($\leftrightarrow$) in Fig 1.10 means
  not flipping back and forth
  not one single + one double bond
  but an average of the individual structures

- double-headed arrow; equilibrium arrow

  $\rightleftarrows$

1.9 Polar Bonds (극성결합)

H — H vs $\underset{\delta+}{\text{H}} \text{ — } \underset{\delta-}{\text{Cl}}$ or $\underset{+\!\!\longrightarrow}{\text{H — Cl}}$

- Atoms with different electronegativity (전기음성도)
  - 📖 18, Table 1.2

- Dipole (쌍극자) moment
  - dipole moment (μ) = (charge amount) (distance)
  - 1 D = (10^{-10} esu) (10^{-10} m) = 10^{-20} esu m
  - a vector quantity
  - μ of a molecule = vector sum of bond dipoles
  - affects physical properties & chemical reactions
  - C–H is a nonpolar bond

1.10 Shapes of molecules

Shapes of molecules are determined by actual experiments not by theoretical considerations!

It is Chemistry and Science.

Experiment First, then Theory

There are some rules for the prediction of the shape.

One is VSEPR (valence shell electron pair repulsion) theory

VSEPR (valence shell electron pair repulsion) theory:

Rule 1: Pairs of electrons in the valence shell repel each other

VSEPR (valence shell electron pair repulsion) theory:

Rule 2: Unshared electron pairs repels more

VSEPR (valence shell electron pair repulsion) theory:

Rule 3: Double and triple bonds as one electron pair

1. 11 Dipole Moments

Molecular dipole moments: depends on shape

Dipole moment of Methanol