Review

$\Delta G = \Delta H - T\Delta S$ (2nd law of thermodynamics)

↓

Change in enthalpy
= bond energy

Exothermic ΔG = Negative

Endothermic ΔG = Positive

Bond Energy

Bond	Bond Energy (kcal/mol)
H-C	99
H-O	111
C-C	83
C=O	179
O=O	119

Ex) $CH_4 + 2\ O_2 \xrightarrow{\Delta} CO_2 + 2\ H_2O$ – Exothermic reaction (releases Energy (E))

$\Delta E_{reaction} = \Delta E_{SM} - \Delta E_{pdt}$

For CH_4:

4 x C-H bonds = 4 x 99 = 396 kcal/mol
2 x O=O = 2 x 119 = 238 kcal/mol
ΔE_{SM} = 634 kcal/mol

ΔE_{SM} = sum of bonds broken (enthalpy)

For products:

2 C=O = 2 x 179 = 358 kcal/mol
4 H-O = 4 x 111 = 444 kcal/mol
ΔE_{pdt} = 802 kcal/mol

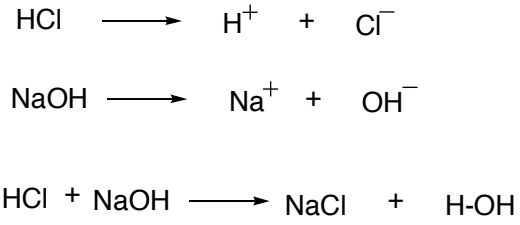
ΔE_{pdt} = sum of bonds formed

$\Delta E_{reaction}$ = 634 kcal/mol – 802 kcal/mol = -168 kcal/mol (exothermic reaction, energy released)

Acids – Bases

- Bronsted – Lowry
  - An acid donates proton (H^+)
  - A base accepts a proton

Ex

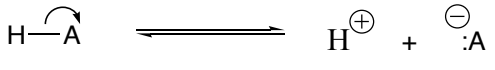


Lewis
- An acid accepts a pair of electrons
- A base donates a pair of electrons

Examples of Lewis acids

H^+ $AlCl_3$ BF_3

Definition

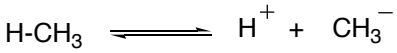


$K_{eq} = K_a = \frac{[H^+][A^-]}{[HA]}$

K_a = acidity constant

$pK_a = -\log K_a$

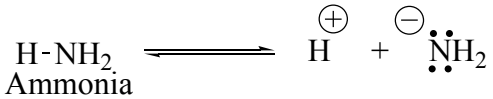
Ex #1)



$$K_a = \frac{[H^+][CH_3^-]}{[HCH_3]} = 10^{-46}$$

$pK_a = -\log K_a = 46$

Ex #2)

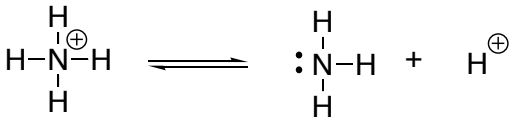


Ammonia gas

$$K_a = \frac{[H^+][^-NH_2]}{[NH_3]} = 10^{-36}$$

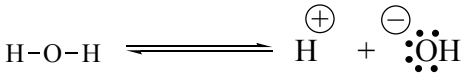
$pK_a = 36$

"pKa of Ammonia" in biological system



Ammonium Cation $pK_a = 9.3$

Ex #3)



$$K_a = \frac{[H^+][^-OH]}{[HOH]} = 10^{-15.7}$$

$pK_a = -\log K_a = 15.7$

Leveling Effect

Strong Acid + Strong Base ⇌ Weak Acid + Weak Base

Ex)

Weak Base — Weak Acid — Stronger Base — Stronger Acid

pKa = 46
Weaker Acid

pKa=16
Stronger Acid

Nomenclature

Learn Names of First 20 Straight Chain Alkanes

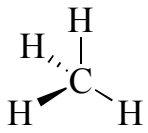
Hydrocarbons – Contain C and H

- Alkanes contain only single bonds (C-H, C-C)
- Alkenes = Olefins C=C
- Alkynes =Acetylenes C≡C

Alkanes

- All carbons are sp^3 hybridized (bond angle of 109^o)
- Held together by London (dispersion) forces

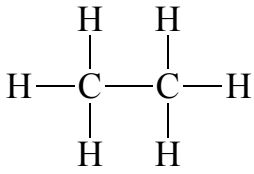
Ex #1) CH_4 , methane



Bp = -161°C

CH_4 H_4C CH_3-H

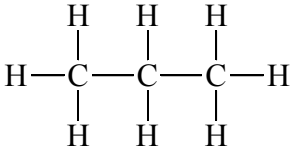
Ex #2) C_2H_6 , ethane



Bp = -88°C

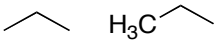
C_2H_6 CH_3-CH_3 H_3C-CH_3

Ex #3) C_3H_8 , propane

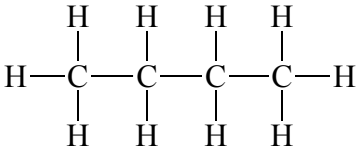


Bp = -42°C

C_3H_8 $CH_3CH_2CH_3$



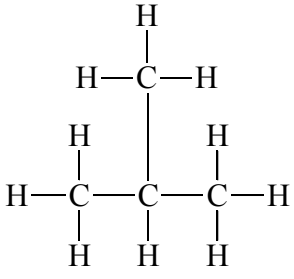
Ex #4) C_4H_{10} , butane



C_4H_{10}, $CH_3CH_2CH_2CH_3$

n-Butane: normal straight chain butane

Ex #5) C_4H_{10} , isobutane

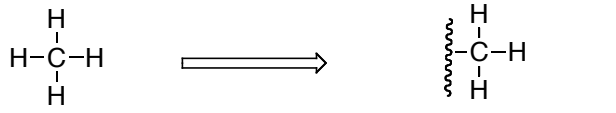


- Isomers (structural or constitutional) are different compounds that have same molecular formula. They have different physical properties (e.g. mp, bp, odour, biological effects)
- Iso - meros
  same - parts

Groups (part of an alkane structure)

- in naming the particular group, drop the "ane" part and add "yl" to the name
- for example, methane → methyl

(i) Methane – CH_4



methane methyl group

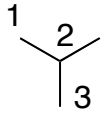
(ii) Ethyl group $-CH_2CH_3$

Systematic Nomenclature

RULES:

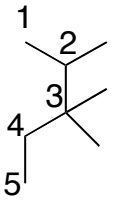
1. find the longest chain with maximum number of branches
2. number from end of the chain, so 1st branch point has lowest number
3. name the chain, then add prefixes (for the groups attached) with number and name the groups attached

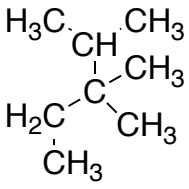
Ex#1)



isobutane (common name)
2-methylpropane (systematic name)

Ex #2)

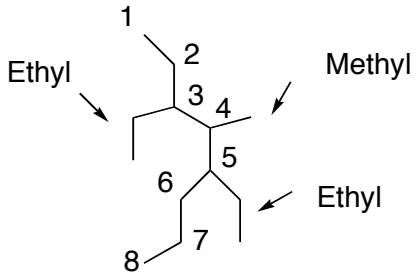




5 Carbon = pentane

2, 3, 3, -trimethylpentane

Ex#3)



3,5-diethyl-4-methyloctane

General Molecular Fomula of Alkanes

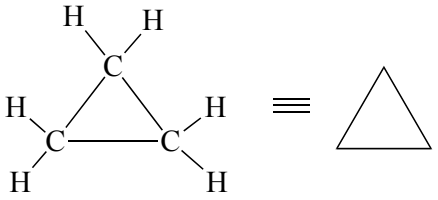
- No rings: general formula is C_NH_{2N+2}
- Each deviation of 2 hydrogens from the C_NH_{2N+2} formula is a degree of unsaturation
- 1 Ring : C_NH_{2N}
- 2 Rings : C_NH_{2N-2}

Ring Structures and Naming:

- start with numbering at point of maximum branches

Cycloalkanes

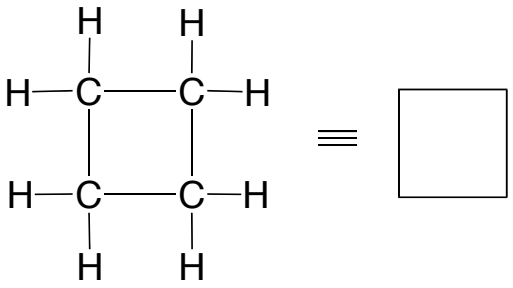
Ex #1) Cyclopropane, C_3H_6



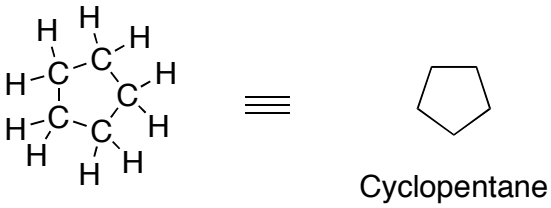
≡

- C-C-C Bond angle (^{o}60)
- Highly reactive due to angle strain.

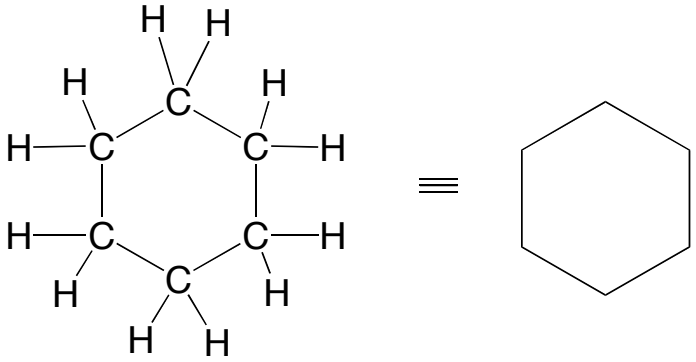
Ex #2) Cyclobutane, C_4H_8



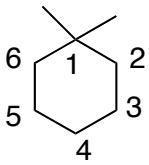
Ex #3) Cyclopentane, C_5H_{10}



Ex #4) Cyclohexane, C_6H_{12}

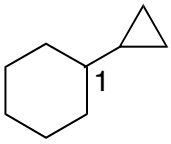


Ex#5)

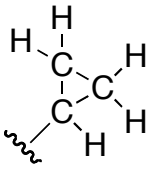


1,1-dimethylcyclohexane

Ex#6)

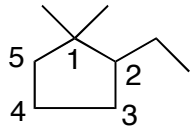


1-cyclopropylcyclohexane



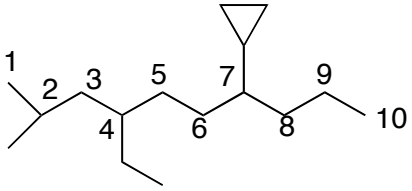
Cyclopropyl

Ex#7)



1,1- dimethyl-2-ethylcyclopentane

Ex#8)



4-ethyl-2-methyl-7-cyclopropyldecane