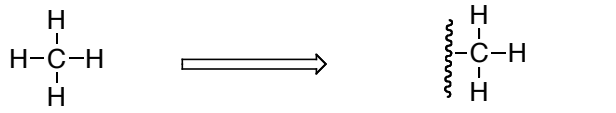
Groups (part of an alkane structure)

- 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 $-CH_2CH_3$

(iii)

iso-propyl group iso-propyl alcohol

(iv)

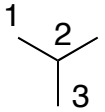
n-propyl chain n-propyl alcohol

Systematic Nomenclature

RULES:

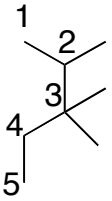
1. find the longest chain with maximum number of branches
2. number from end of the chain, so 1st branch point has lowest number
3. name the chain, then add prefixes (for the groups attached) with number and name the groups attached

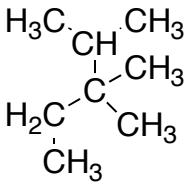
Ex#1)



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

Ex #2)

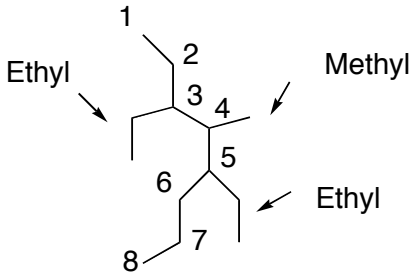




5 Carbon = pentane

2, 3, 3, -trimethylpentane

Ex#3)



3,5-diethyl-4-methyloctane

General Molecular Fomula of Alkanes

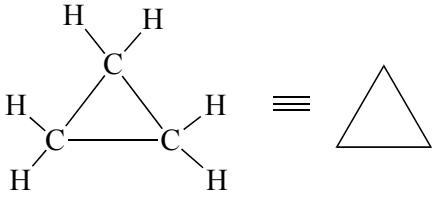
- No rings: general formula is C_NH_{2N+2}
- Each deviation of 2 hydrogens from the C_NH_{2N+2} formula is a degree of unsaturation
- 1 Ring: C_NH_{2N}
- 2 Rings: C_NH_{2N-2}

Ring Structures and Naming:

- start with numbering at point of maximum branches

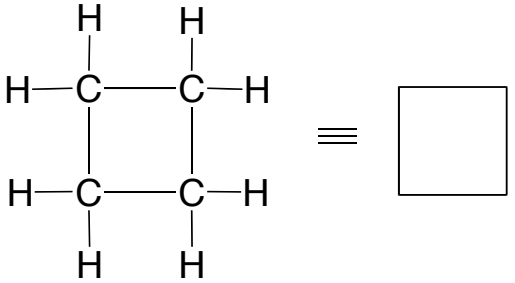
<u>Cycloalkanes</u>

Ex #1) Cyclopropane, C_3H_6

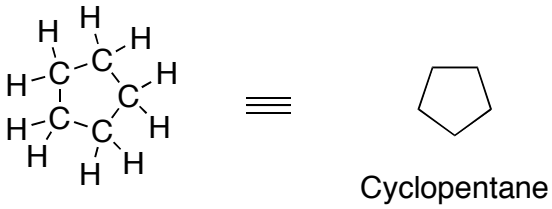


- C-C-C Bond angle (^{o}60)
- Highly reactive due to angle strain.

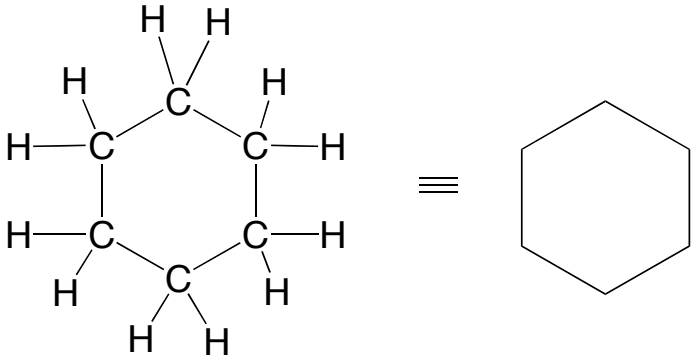
Ex #2) Cyclobutane, C_4H_8



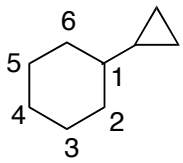
Ex #3) Cyclopentane, C_5H_{10}



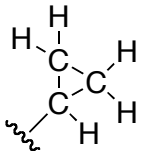
Ex #4) Cyclohexane, C_6H_{12}



Ex#5)

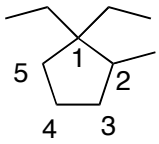


1-cyclopropylcyclohexane



Cyclopropyl

Ex#6)

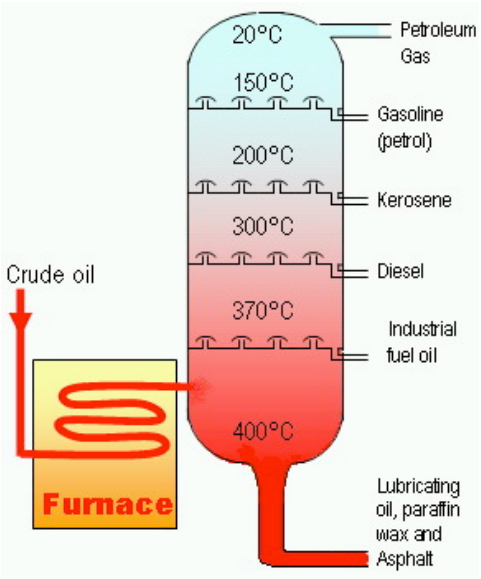


1,1-diethyl-2-methylcyclopentane

Physical Properties:

- hydrocarbons – alkanes are non-polar – H and C have similar electronegativity therefore there is no permanent dipole
- soluble in other organic solvents (like dissolves like)
- immiscible with water (not infinitely soluble in water)

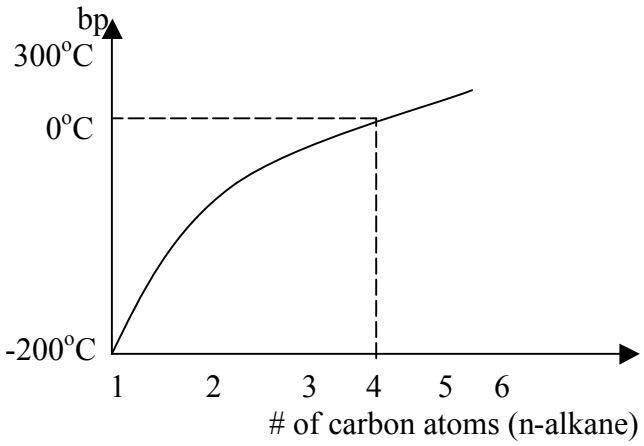
Distillation of petroleum



cold

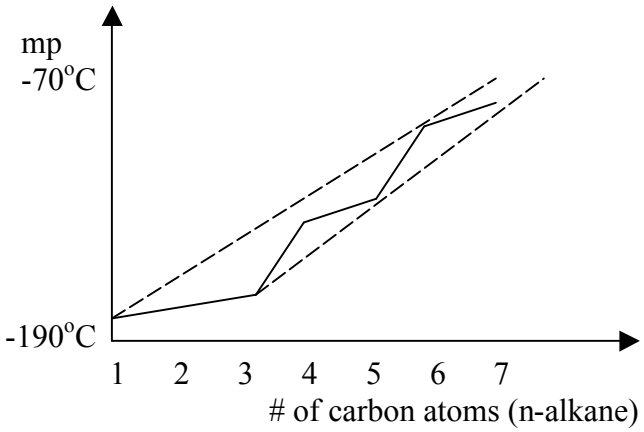
hot

boiling point trend:

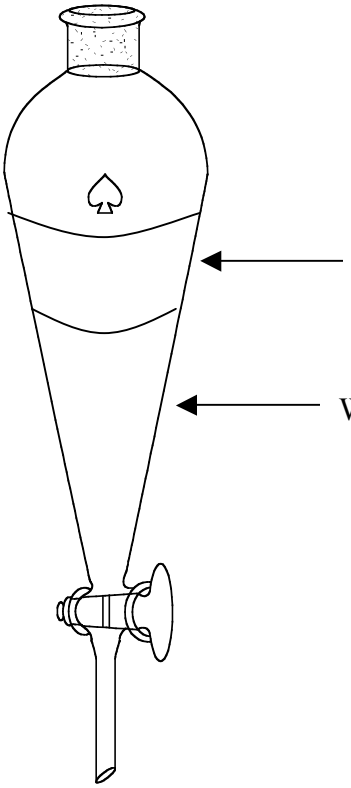


- increasing the straight chain length increases the bp. This is due to London forces (hydrophobic forces) between the adjacent molecules.

melting point trend:



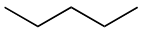
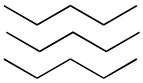
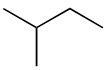
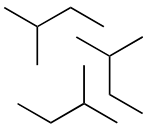
- melting points are related to the crystal structure packing efficiency



Alkanes are less dense than water (0.65-0.75 g/mL)

Water (1.0 g/mL)

eg. pentane

	mp (^{o}C)	bp (^{o}C)	
	-129	36	well packed 
	-160	28	 less well packed
	-13	9	"ball-like" shape, so B.P. comes down

- n-pentane has high bp due to multiple contacts of straight chains (London Forces)
- melting point of neopentane determined by good crystal packing of spherical shape

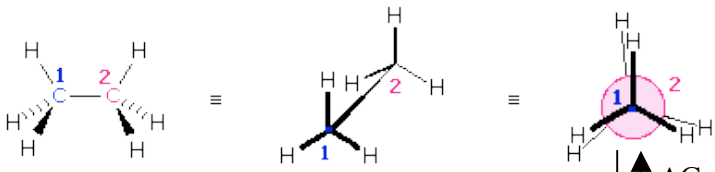
Conformations

- Different 3-D shapes a molecule can assume by rotation around single bonds.

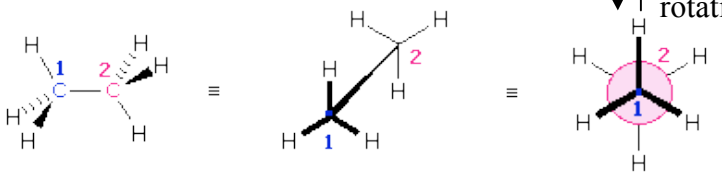
Eg) ethane – C_2H_6

Newman projection

Less stable Eclipsed Conformation



Most stable Staggered Conformation



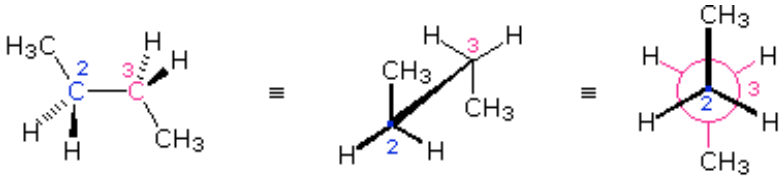
ΔG = 2.8 kcal/mol for rotation

- Rotation occurs rapidly at room temperature.
- Room temperature = ~15-20 kcal/mol of energy available.

Eg) n-butane (C_4H_{10}) – rotation around all bonds still very rapid

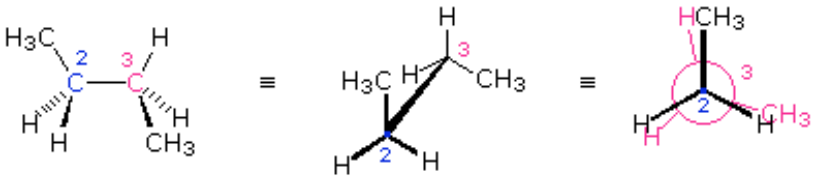
- most stable (most populated conformation) is called anti and has groups as far away as possible

A



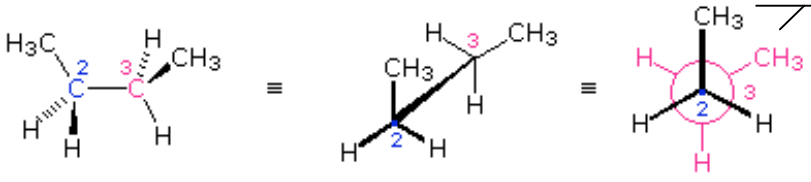
Anti Conformation — Most stable, staggered Dihedral angle = 180°

B



Eclipsed Conformation — Dihedral angle = 120°

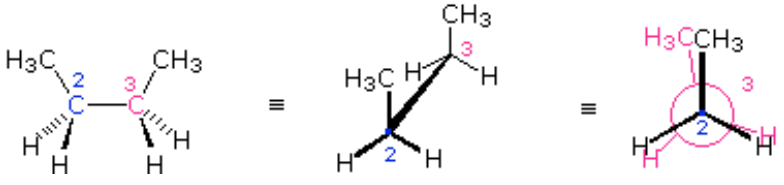
C



Repulsion = steric effect

Gauche Conformation — Not as stable as anti Dihedral angle = 60°

D



Eclipsed Conformation — Least stable (syn) Dihedral angle = 0°

The dihedral angle in the above diagram is the angle between the two methyl groups.