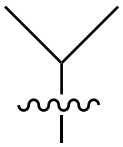
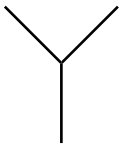
Systematic Nomenclature

RULES:

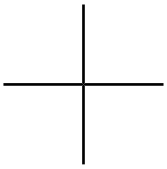
1. Find the longest chain
2. Number from end of the chain, so that the 1st branch point has the lowest number
3. Name the chain, then add prefixes (for the groups attached) with number and name the groups attached
4. Separate numbers and names by dash



isopropyl



isobutane
2-methylpropane

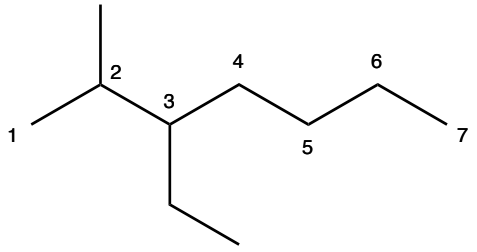


neopentane
2,2-dimethylpropane

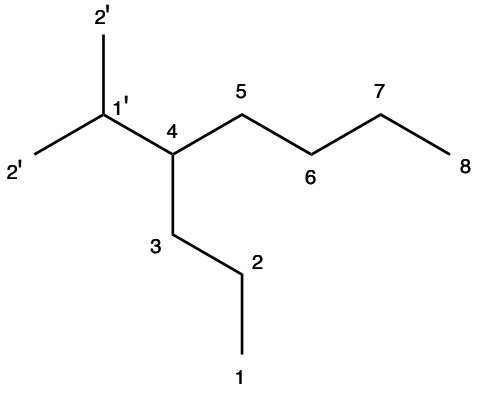
Note: iso = second-to-last carbon of the chain is disubstituted (2 methyl groups)
neo = second-to-last carbon of the chain is trisubstituted (3 methyl groups)

Recall: CH_2 – methylene group, CH_3 – methyl group

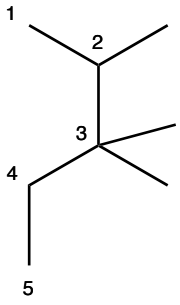
Examples



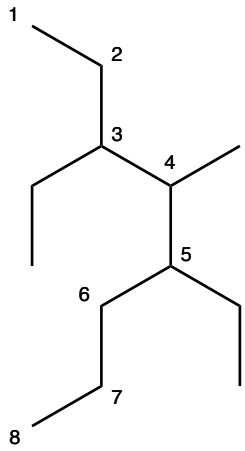
3-ethyl-2-methylheptane



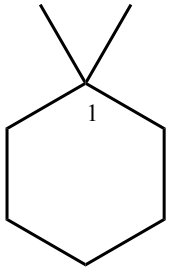
4-(1-methylethyl)octane



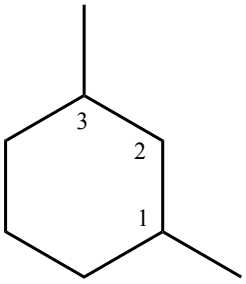
2,3,3-trimethylpentane



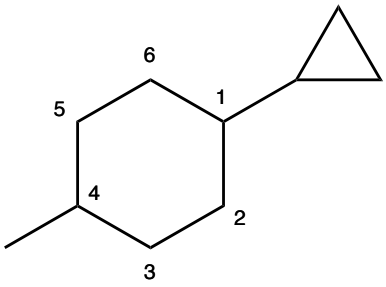
3,5-diethyl-4-methyloctane



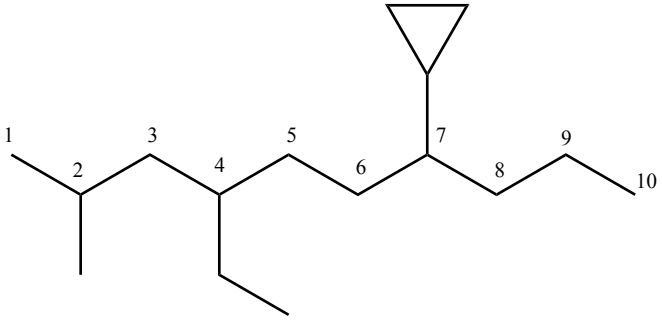
1,1-dimethylcyclohexane



1,3-dimethylcyclohexane



1-cyclopropyl-4-methylcyclohexane
- A disubstituted cycloalkane

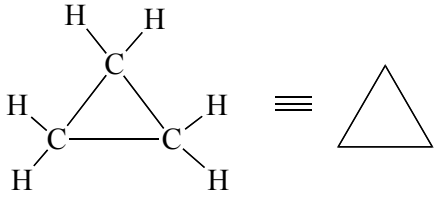


7-cyclopropyl-4-ethyl-2-methyldecane

Note: Ring Structure Naming
- Prefix with "cyclo"
- Start with numbering at point of maximum branching/most important functional group
- Number so as to give next branch/functional group lowest number

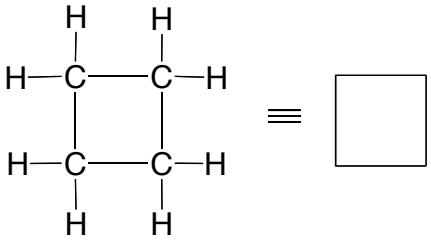
Cycloalkanes

Cyclopropane, C_3H_6

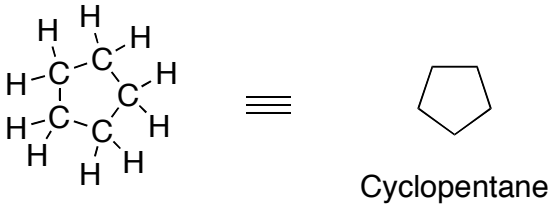


- One degree of unsaturation (n-propane is C_3H_8)
- C-C-C bond angle (60 ^{o})
- Highly reactive due to ring strain

Cyclobutane, C_4H_8

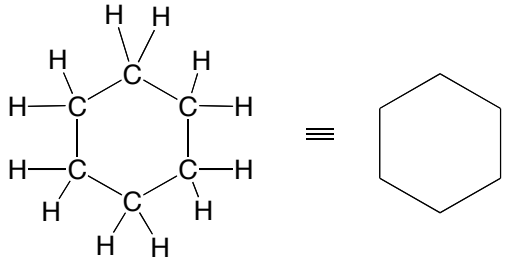


Cyclopentane, C_5H_{10}



Cyclopentane

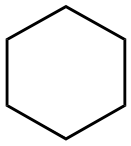
Cyclohexane, C_6H_{12}



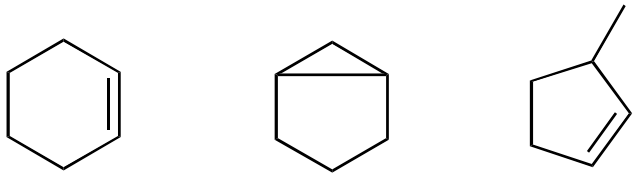
General Molecular Formula of Alkanes

- 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 Degree of unsaturation : C_NH_{2N} Alkanes with one ring or double bond
- 2 Degrees of unsaturation : C_NH_{2N-2} Alkanes with two rings or double bonds, or one each

Examples



C_6H_{12} 1 degree of unsaturation



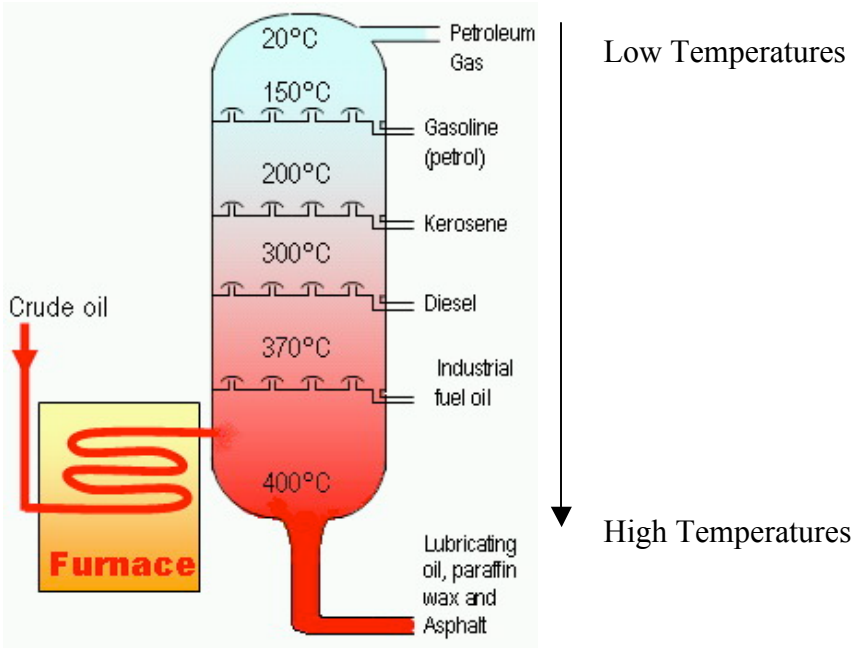
C_6H_{10} 2 Degrees of unsaturation

The above three are structural (constitutional) isomers

Source of Hydrocarbons

- Petroleum *(John D. Rockefeller)*

Distillation of Petroleum:

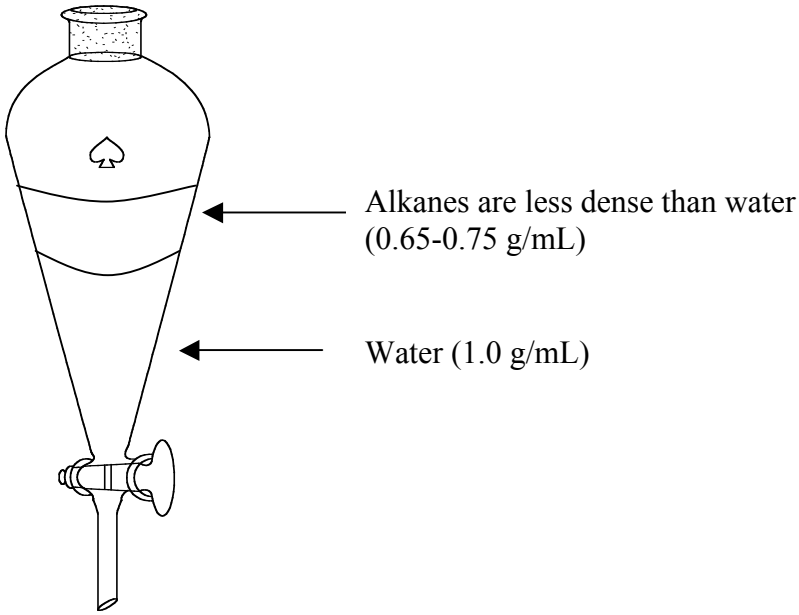


- Petroleum is a mixture of alkanes and other hydrocarbons (>>500 compounds)

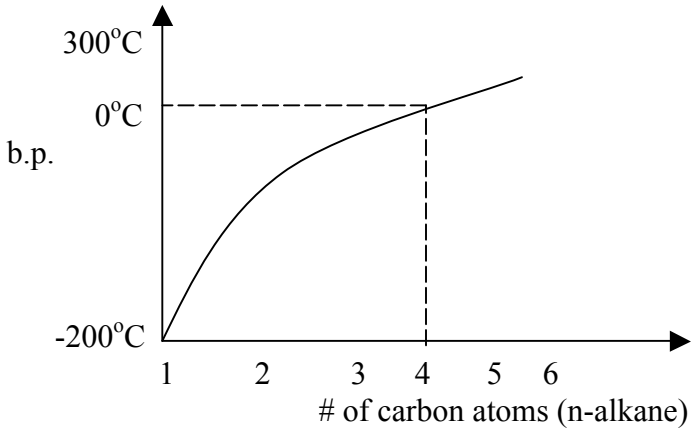
Physical Properties of Alkanes:

- Intermolecular forces are dominated by London forces
- Alkanes are non-polar because H and C have similar electronegativity
- Soluble in other organic solvents (like dissolves like)
- Not miscible with water → floats due to lower density
- Low density (ρ = rho = g/cm^3)
    - ρ water ~ 1 g/cm^3
    - ρ alkanes ~ 0.7 g/cm^3
- Low m.p., b.p.

Separatory Funnel *(density separation)*

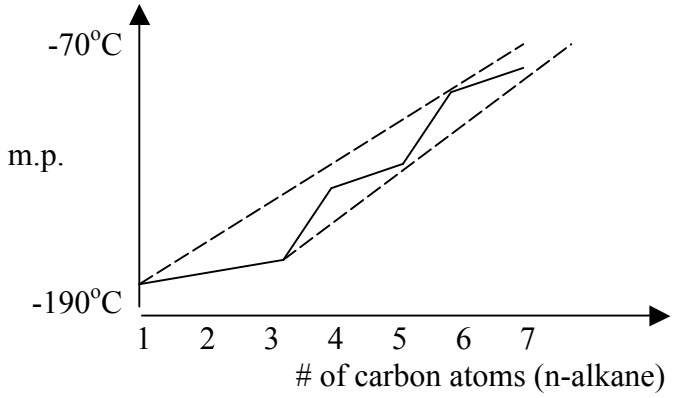


Boiling point trend:



- As the straight chain length increases, so does 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

e.g. Pentane

	mp (°C)	bp (°C)	
n-Pentane	-129	36	well packed
Isopentane 2-methylbutane	-160	28	less well packed
Neopentane 2,2-dimethylpropane	-13	9	"ball-like" shape, so B.P. comes down

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

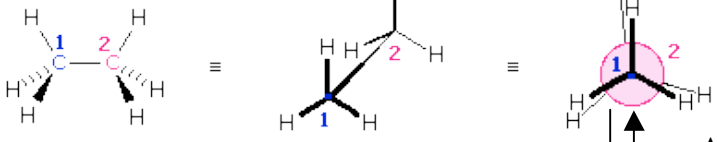
Conformations

- Different 3-D shapes a molecule can assume by rotation around single bonds
- Room temperature (20 °C): 15-20 kcal/mol of energy available
- Rotation around C-C occurs rapidly at room temperature
- Steric effect: Repulsion of filled shells of e^-

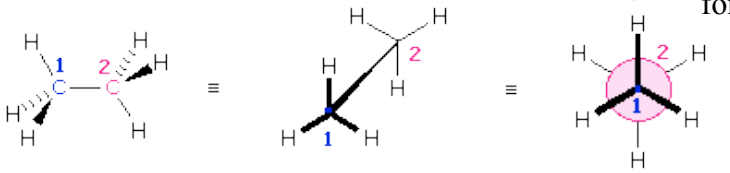
Ethane (C_2H_6)

Newman Projection

Less stable — Eclipsed Conformation



Most stable — Staggered Conformation

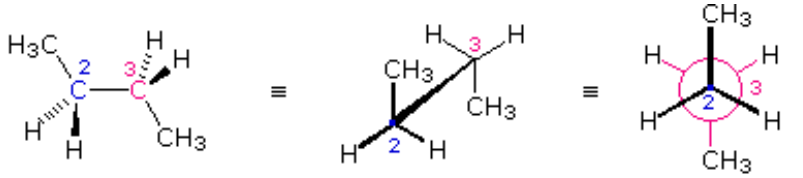


ΔG = 2.8 kcal/mol for rotation

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

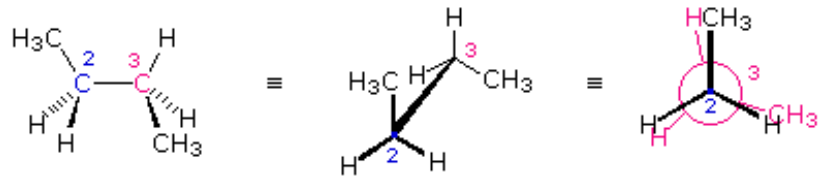
- Most stable (most populated conformation) is called anti and has groups as far away as possible

A



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

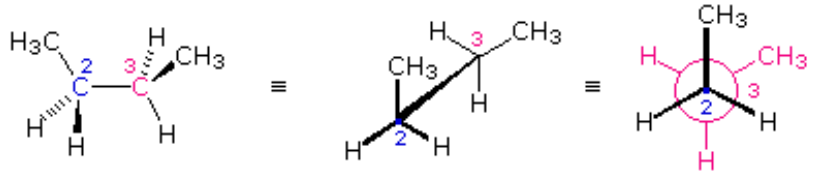
B



Eclipsed Conformation — Dihedral angle = 120°

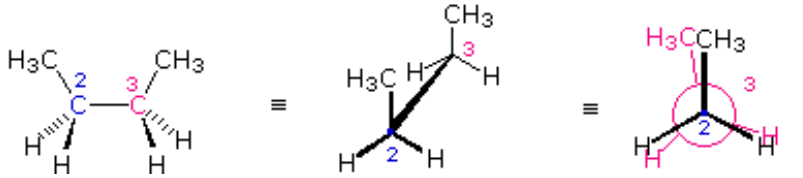
Repulsion = steric effect

C



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

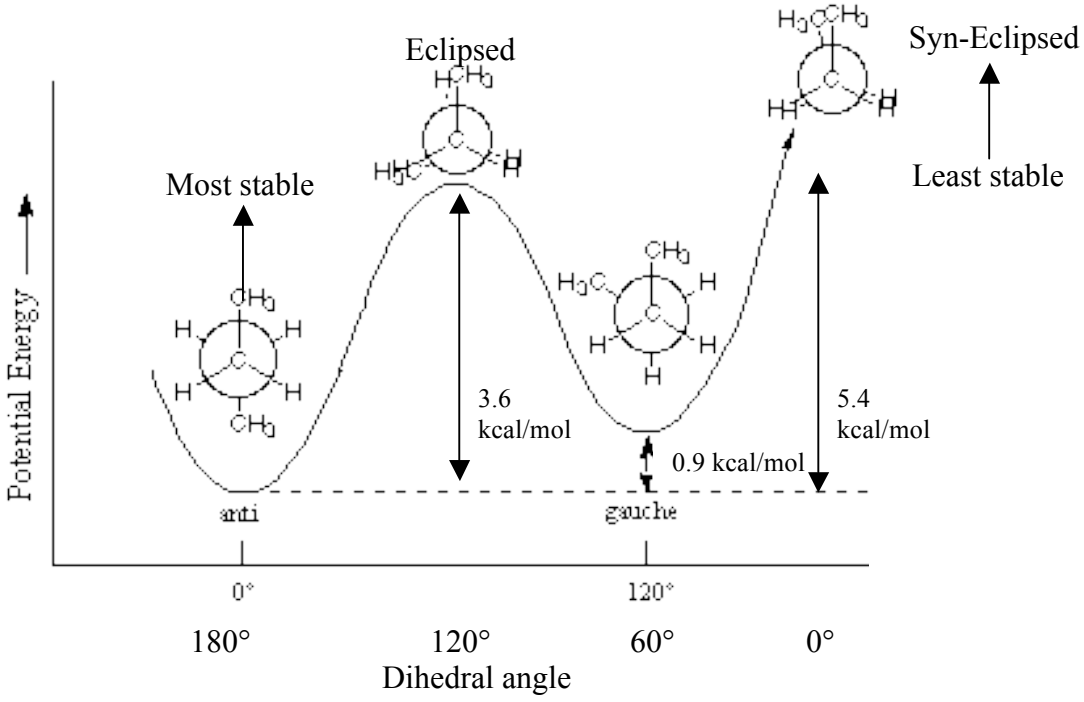
D



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

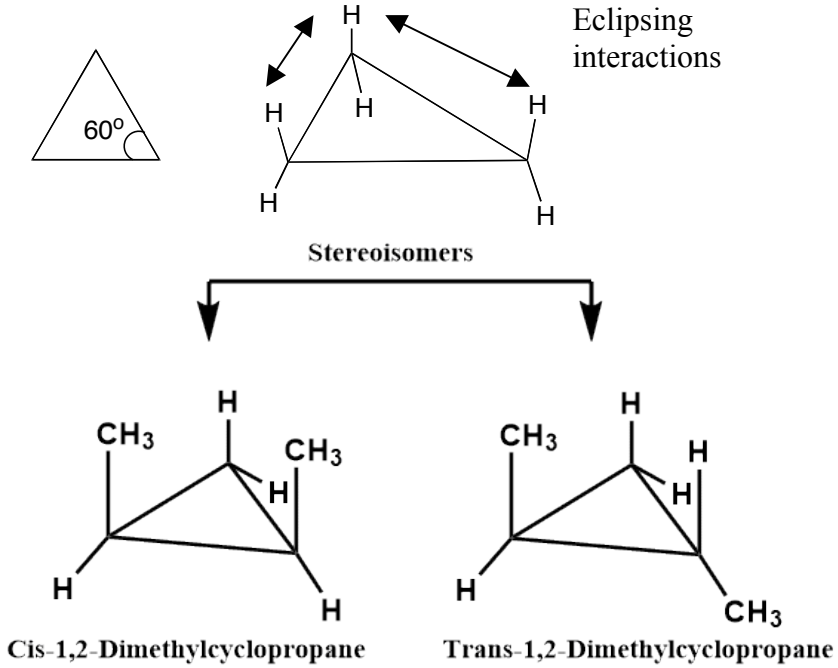
Energy diagram

- The dihedral angle is the angle between the two-methyl groups.

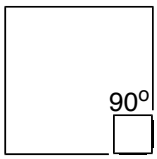


Cycloalkane Conformations

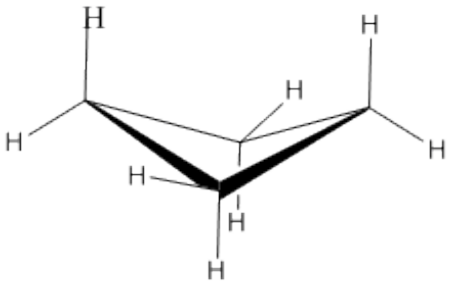
Cyclopropane –bond angle 60^{o} – relatively rigid structure



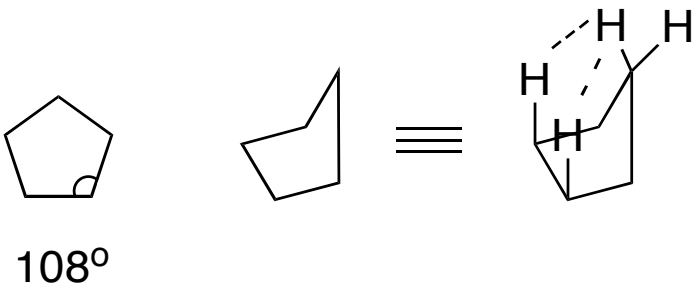
Cyclobutane – bond angle close to 90^{o} – does have some flexibility



3D structure



Cyclopentane – bond angles nominally 108^{o} – more flexible than cyclobutane



Cyclohexane – bond angles actually 109^{o}, not 120^{o} as in flat hexagon