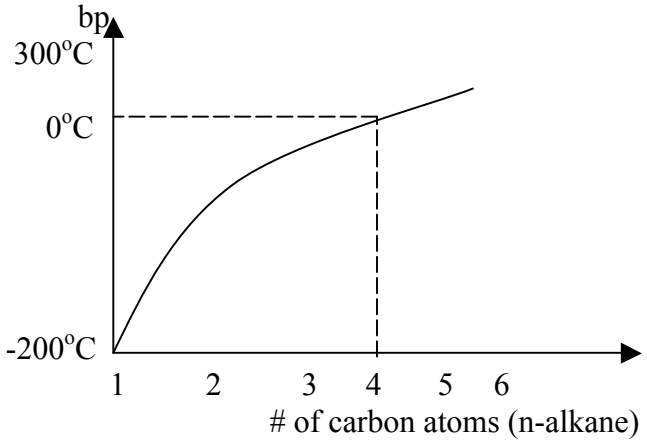
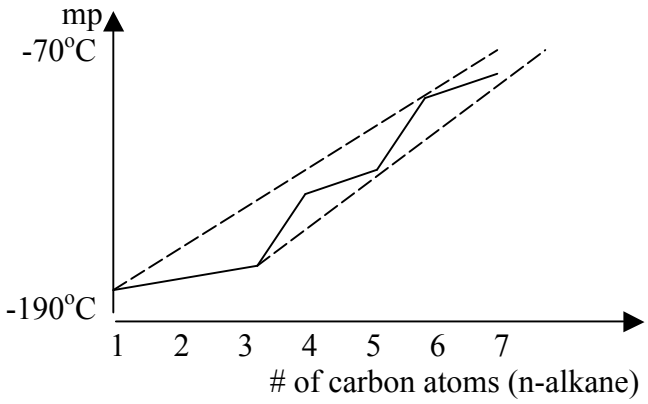
Alkanes – Physical Properties Continued

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:



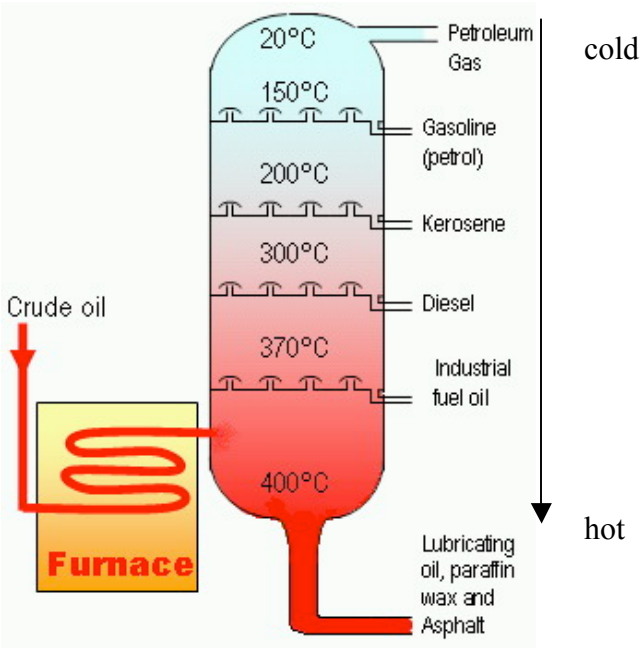
- Melting points are related to the crystal structure packing efficiency

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

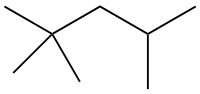
- n-pentane has high bp due to multiple contacts of straight chains (London Forces)
- mp of neopentane determined by good crystal packing of spherical shape

Distillation of Petroleum

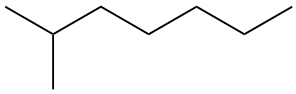


- Petroleum is a mixture of alkanes and other hydrocarbons (>>500 compounds)

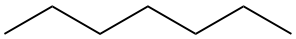
Octane Rating



"isooctane" = 2,2,4-trimethylpentane
Defined as having an octane rating of 100



isooctane

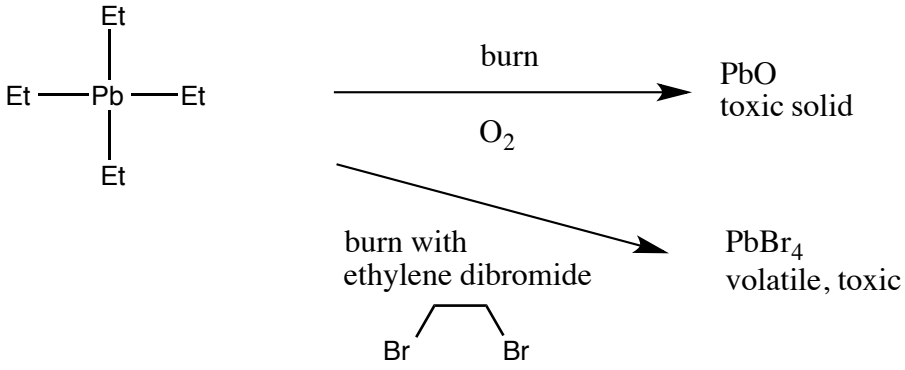


n-heptane
poor octane

90 octane rating – "Knock" is like 90:10 mixture of "isooctane" / n-heptane

Leaded gasoline

- Tetraethyl lead used to be added to gasoline as an antiknock compound
- Ethylene dibromide also used to be added to leaded gasoline

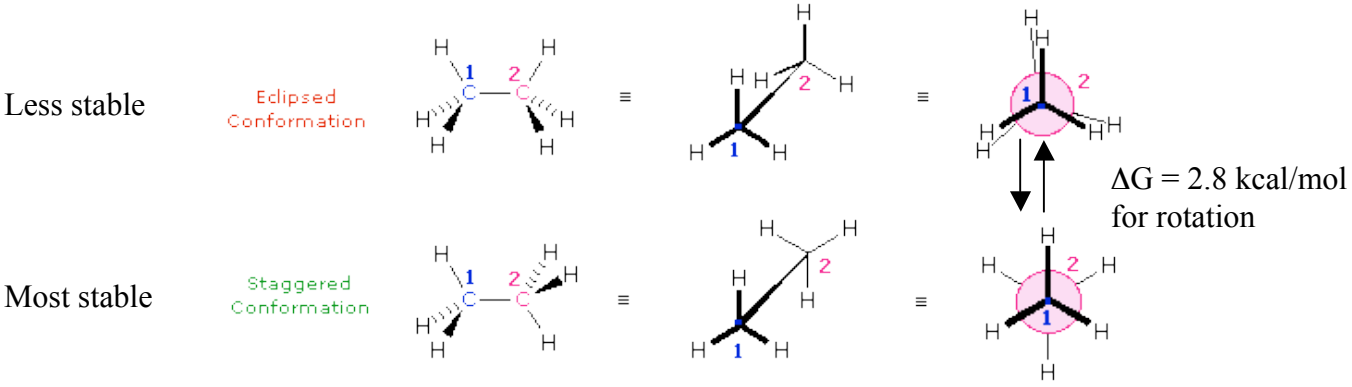


Conformations

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

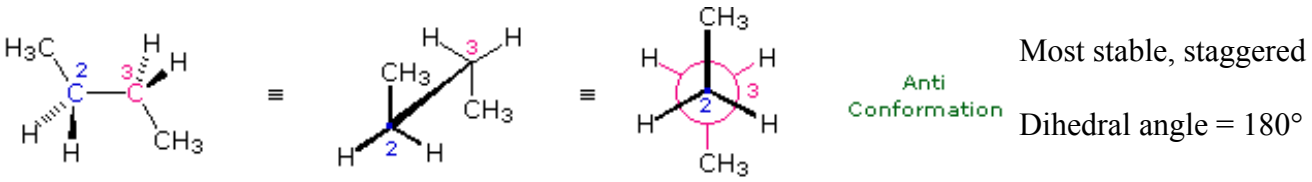
Ethane (C_2H_6)

Newman Projection



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

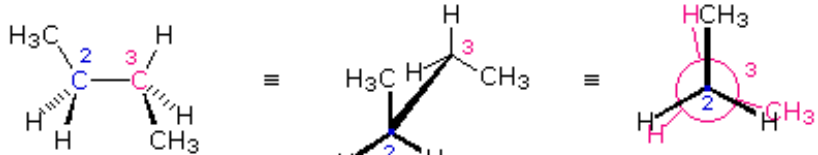
- Most stable (most populated conformation) is called anti and has groups as far away as possible

A 

Anti Conformation

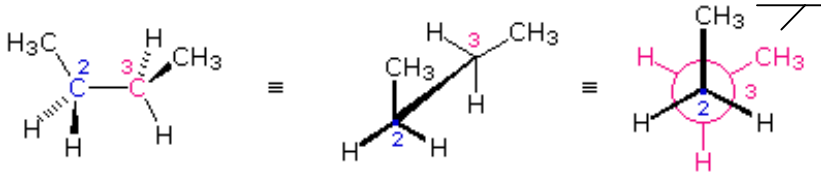
Most stable, staggered

Dihedral angle = 180°

B 

Eclipsed Conformation

Dihedral angle = 120°

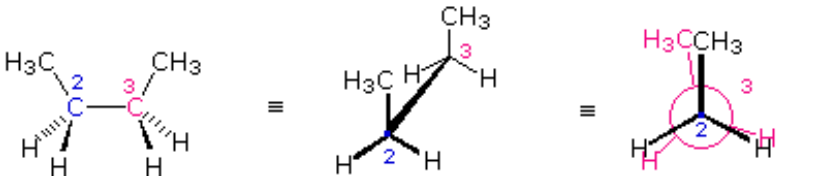
C 

Repulsion = steric effect

Gauche Conformation

Not as stable as anti

Dihedral angle = 60°

D 

Eclipsed Conformation

Least stable (syn) eclipsed

Dihedral angle = 0°