

Chap 4

3 Rxn factors

1. Mechanism- step by step description of the movement of e' and atoms.
2. Thermodynamics- energy changes
3. Kinetics- reaction rates

Gibbs free energy

$$\Delta G = \Delta H - T\Delta S$$

$\Delta G = (+)$ non-spon., $(-)$ spon.

$\Delta H =$ enthalpy heat energy, $(-)$ exothermic, $(+)$ endothermic

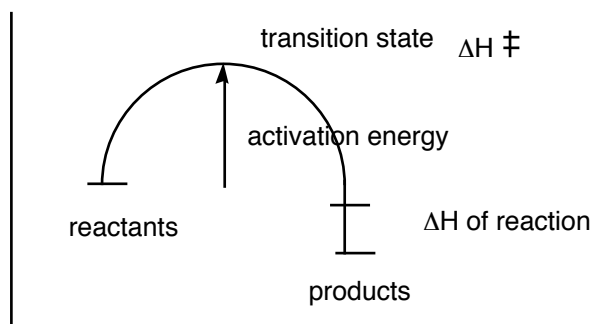
$\Delta S =$ entropy (disorder), $(+)$ more disorder, $(-)$ less disorder

$T =$ related to kinetic energy

favorable – $(-)$ enthalpy, $(+)$ entropy, high T

Activation energy- minimum kinetic energy needed to overcome repulsion.

$$K = Ae^{-E_a/RT} \quad \text{rate} = k[A]^x[B]^y \quad A = \text{constant} \quad K = \text{rate constant}$$



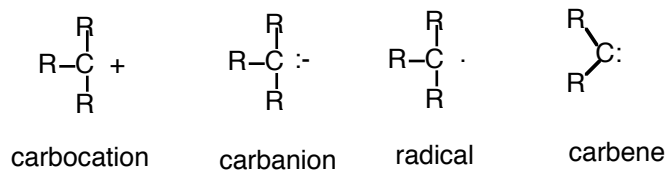
Catalyst- lowers activation energy.

Transition state- highest energy state in a molecular collision.

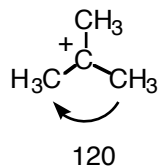
Intermediate- isolatable.

Reactive Intermediates-

Ex. For carbon.

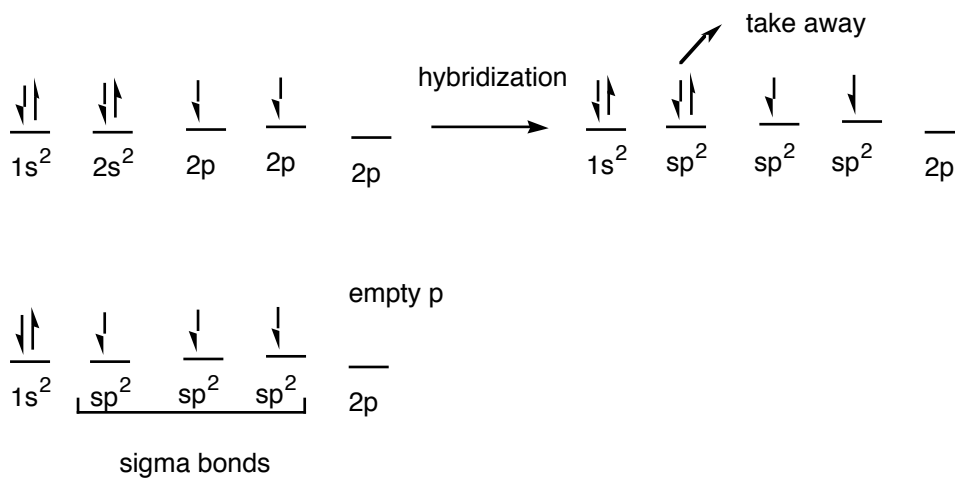
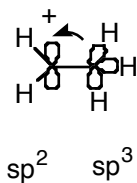


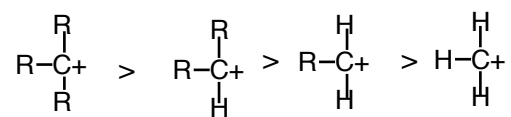
1. carbocation- sp^2 hybridized trig planar geometry, no stereochem



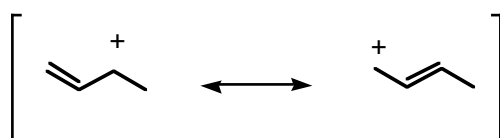
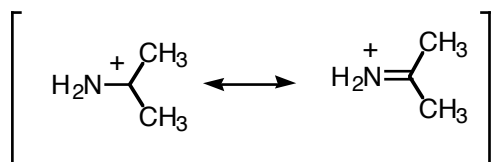
alkyl groups are e^- donating by:

- A) Inductive effects. Donation of e^- through sigma bonds, through space.
- B) Hyperconjugation, overlap between a p orbital and a sigma bond.



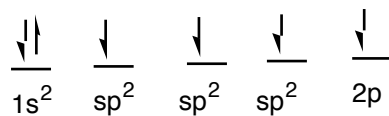
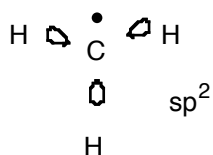


c) Resonance stabilization.



2. Free Radicals-

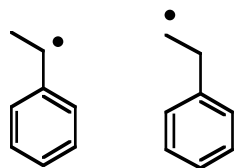
120- trigonal planar



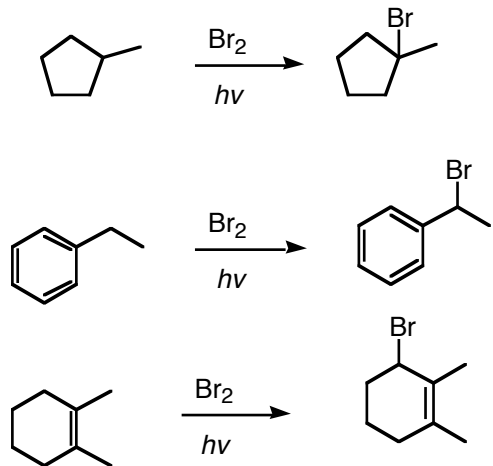
lone e'

a) stability same as carbocation because e' deficient.

Most stable?

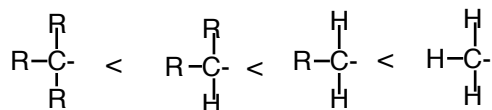


Free radical Bromination:

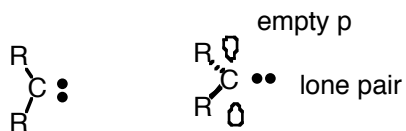


3. Carbanions- negative charge on carbon.

Alkyl groups e' donating. Destabilize negative charge.



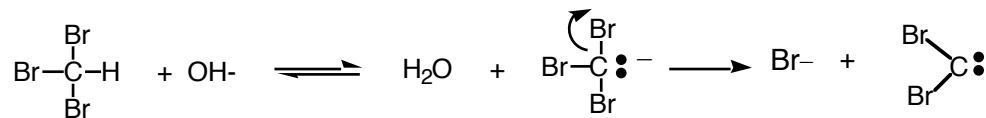
4. carbenes- neutral species with deficient e' but pair.



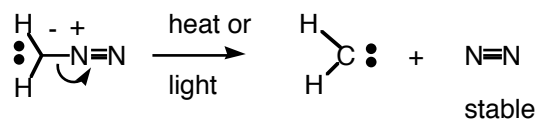
lone pair can act as a nucleophile or electrophile. Lewis acid or base.

Formation of carbenes,

a) Br make H more acidic because of EN.



b)



c) Use of carbenes. Insertion into alkenes to make cyclopropanes.

