CHEM 261 Oct 04, 2017

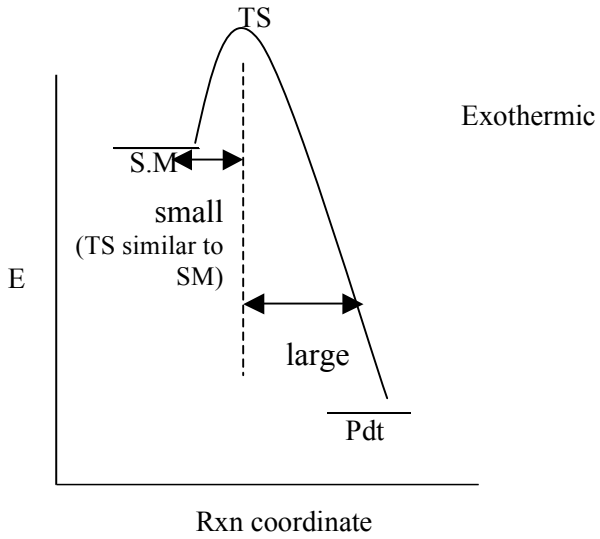
Review from last class:

Reactivity vs Selectivity (Halogenation)

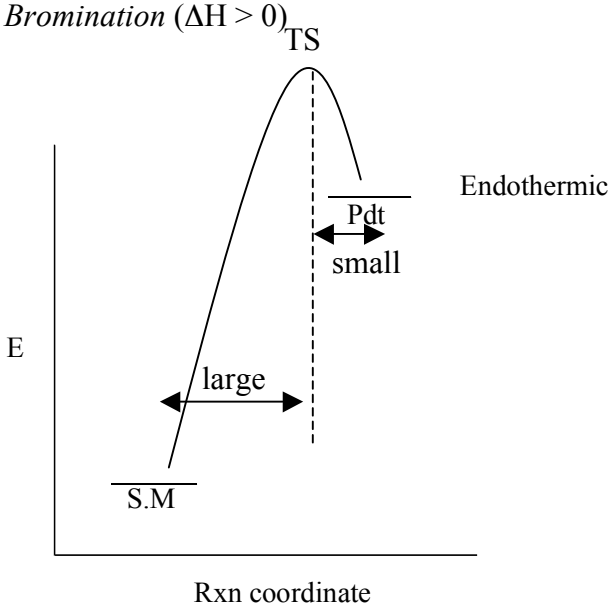
F >> Cl > Br > I

Energy Diagrams for Halogenation Reactions

Chlorination (ΔH < 0)



Bromination (ΔH > 0)

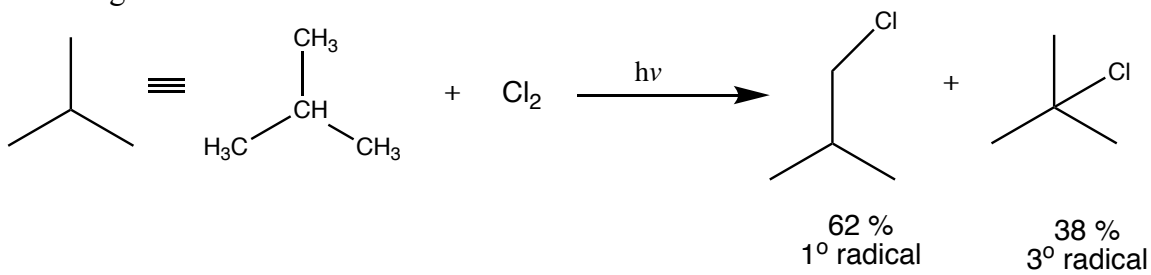


E = energy (kcal/mol) Pdt = product

TS = transition state

SM = starting material

Other examples: How many times more reactive is the most stable radical considering the following reaction-outcome?

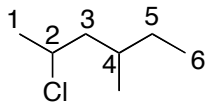


- for the 1° radical product, there are 9 hydrogen atoms (3 × C<u>H</u>$_3$) that can be substituted by chlorine, therefore the 62% will be divided by those 9 atoms (62:9 =~7)
- for the 3° radical product, there is only one hydrogen atom (1 x C<u>H</u>) that can be substituted by chlorine, therefore the 38% probability will be divided by 1 H atom (38:1=38)
- Calculating the relative probability ratio between the two radicals (38/7= 5.5), the 3° radical is 5.5x more reactive than the 1° radical.

Alkyl Halides = Haloalkanes

Structure and Nomenclature

1) Find longest chain with largest number of branches
2) Number from end so as to give 1st branch the lowest number
3) Name prefix with "halo" (chloro, bromo, iodo, fluoro) OR name alkyl and add halide (chloride, bromide, iodide, fluoride) as the suffix

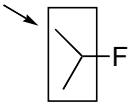


2 -chloro -4-methylhexane

Fluorocyclopropane

Cyclopropyl fluoride

Isopropyl

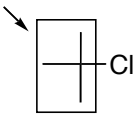


2-Fluoropropane

2-Propylfluoride

Isopropyl Fluoride

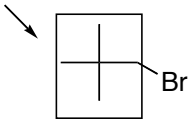
tert-Butyl



2-Chloro-2-methylpropane

tert-Butyl Chloride

Neopentyl



Neopentyl Bromide

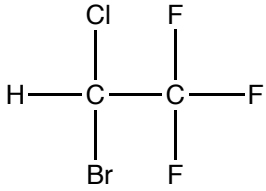
1-Bromo-2,2-dimethylpropane

Physical Properties of Alkyl Halides:

- Governed primarily by dipole-dipole interactions.
- "Non-polar", but more polar than hydrocarbons.
- High MP and BP relative to hydrocarbons of similar molecular weight
- Good solvents for organic compounds e.g. Methylene chloride (CH_2Cl_2) and chloroform ($CHCl_3$) are very common.
- Density = ρ (rho) = 1.0 g/cm^3 (similar to water's)
- If % composition > 65% halogen by weight, then more dense than water (ρ > 1.0)
- Immiscible (insoluble) in H_2O, which floats on top of the halide.

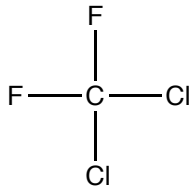
Applications of Haloalkanes

1. Halothane (anesthetic)

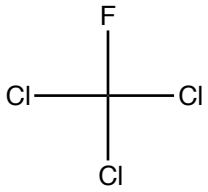


1,1,1-trifluoro-2-bromo-2-chloroethane

2.) Freon = refrigerants/coolants

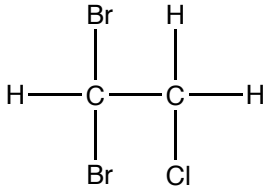


Freon 12



Freon 11

3.) 1,1-dibromo-2-chloroethane = male sterilizer (sperm count drops down to zero)



Introduction to Stereochemistry and Chirality (terminologies)

Chiral (greek:'hand') object or molecule: has a non-superimposable mirror image
Achiral object: not chiral, has a superimposable mirror image

Enantiomers: molecules that are stereoisomers and are non-superimposable mirror images of each other

Diastereomers: stereoisomers that are not enantiomers