CHEM 261 Sept 26, 2014

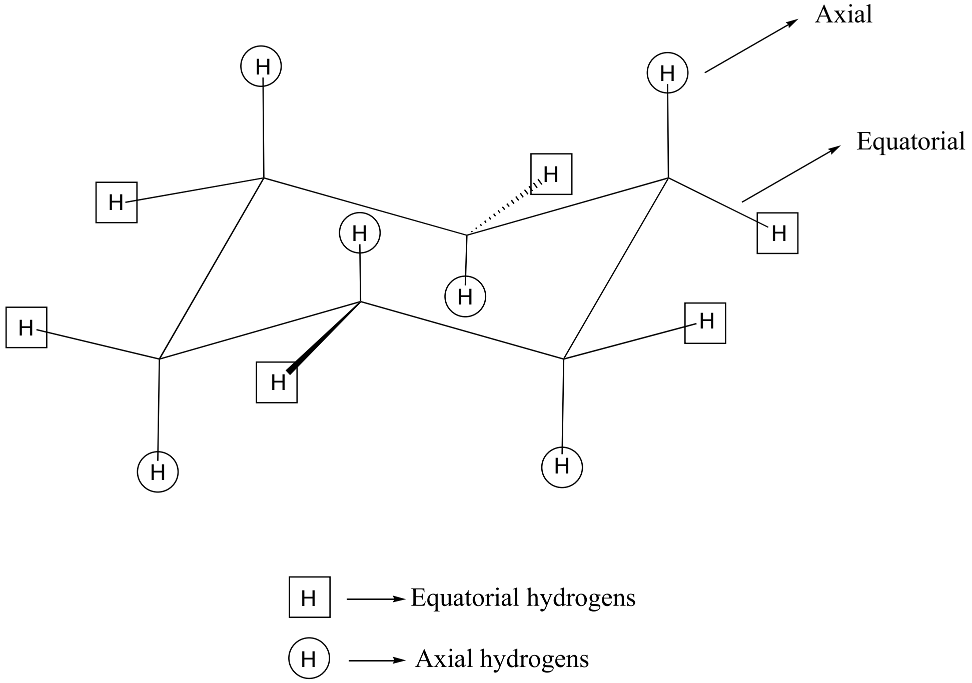
Review

Conformations – different shapes a single molecule may assume via rotation around single bonds

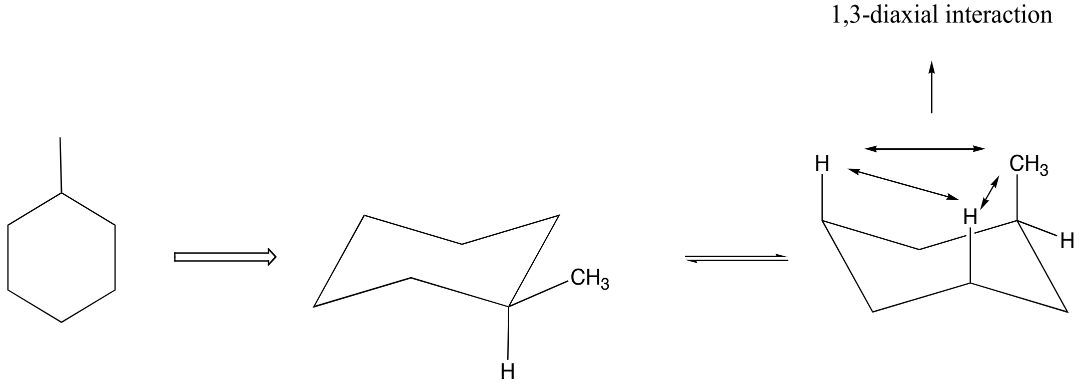
Isomers - different compounds with same molecular formula – 2 basic types

1. Structural/constitutional isomers
   – Compounds with same molecular formula
2. Stereoisomers – same connectivity but different 3-D structure – 2 sub-types
   (a) diastereomers/diastereoisomers (eg. *cis*/*trans*)
   (b) enantiomers (non-superimposable mirror images of same molecule)

Cyclohexane Conformations



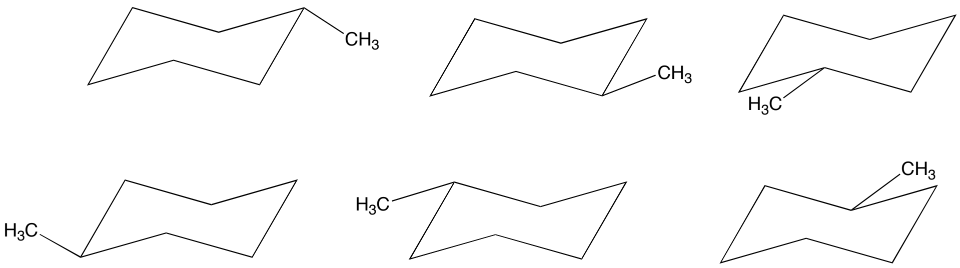
Substituted Cyclohexanes – Draw most stable conformation



- Largest (bulkiest group close to ring) group generally placed equatorial – otherwise get unfavorable 1,3-diaxial interactions

- 1,3-diaxial interaction (steric effect) makes this conformation less stable.

Most Stable Conformation of Methylcyclohexane – 6 drawings of same molecule below

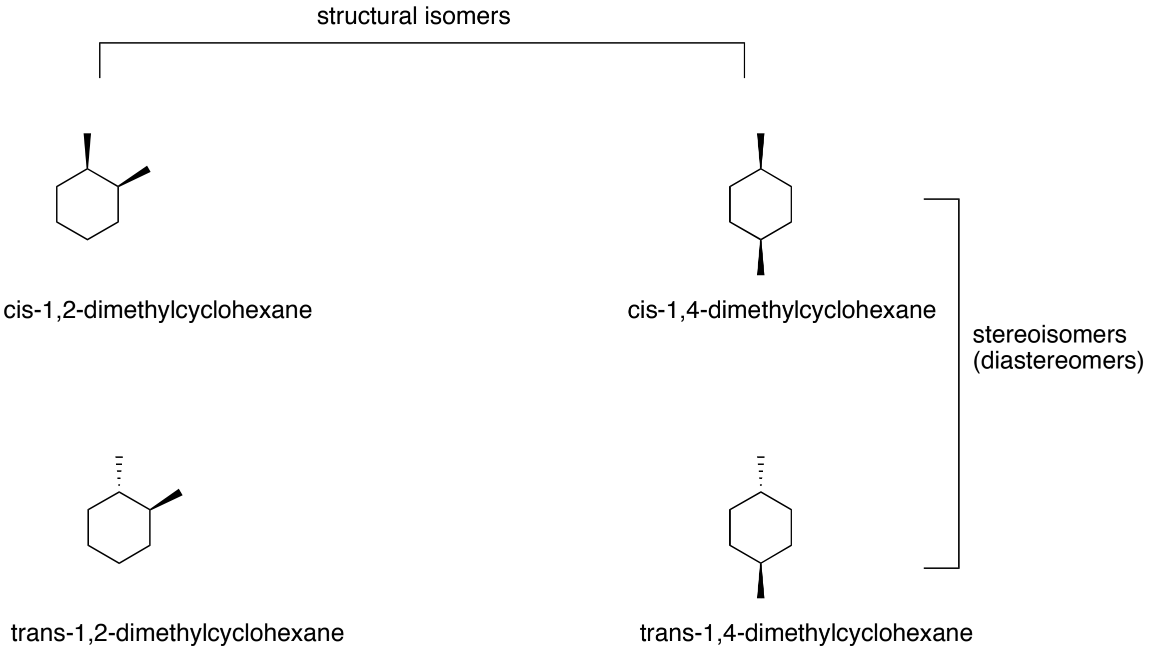


Polysubstituted cyclohexane

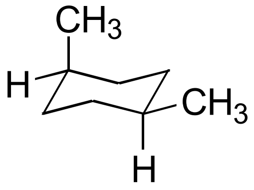
Isomers - different compounds with same molecular formula

Conformers – different shapes of the same molecule

Example: 1,2-dimethylcyclohexane and 1,4-dimethylcyclohexane

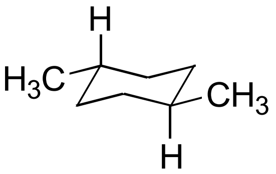


Example: Cis-1,4-Dimethylcyclohexane:



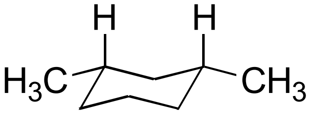
Cis-1,4-Dimethyl Cylcohexane

Example: Trans-1,4-Dimethylcyclohexane:



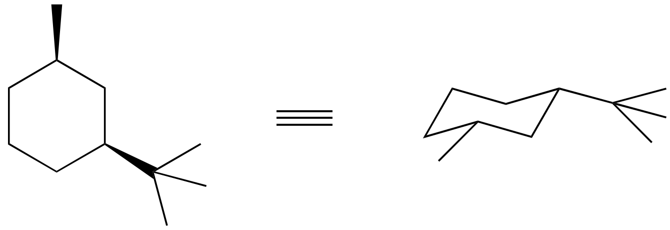
Trans-1,4-Dimethyl Cylcohexane

Example: Cis-1,3-Dimethylcyclohexane:



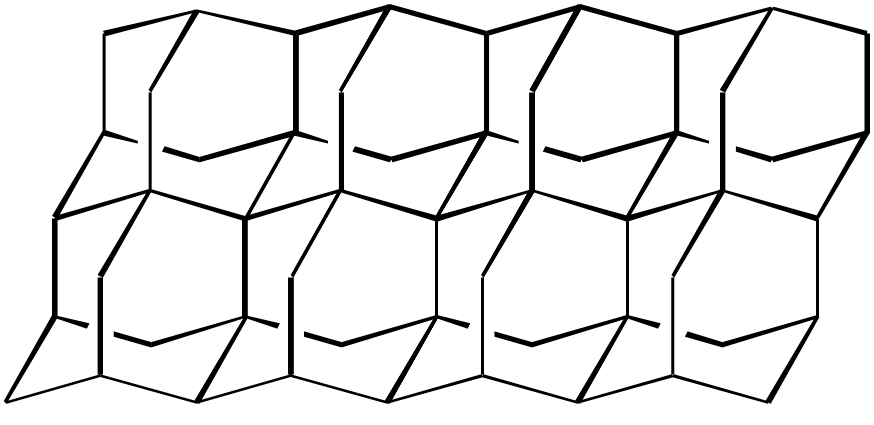
Cis-1,3-Dimethyl Cylcohexane

Example: Cis-1-tert-butyl-3-methyl-cyclohexane



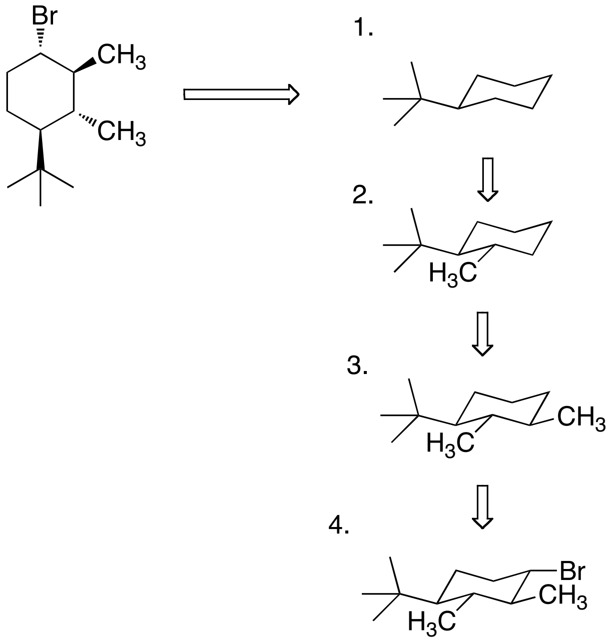
Note that the largest substituent (tert-butyl) is placed in the equatorial position to avoid destabilizing 1,3 diaxial interactions and the methyl is placed *syn* to the tert-butyl group.

Diamond:



Further Example:

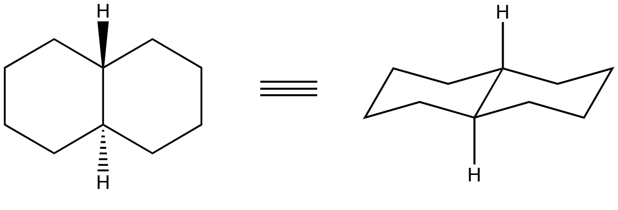
Steps for drawing



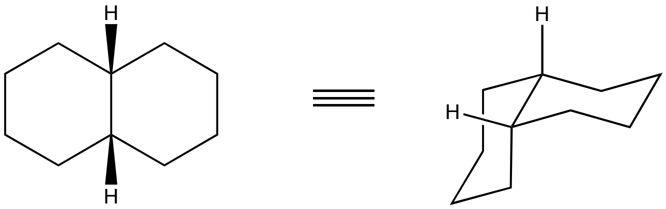
Note on drawing the most stable conformation of substituted cyclohexanes:
- generally, draw chair conformation of cyclohexane
- put the largest group in equatorial position
- draw the next group on the correct side (face) with respect to the largest group

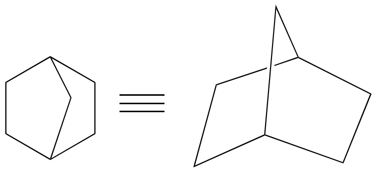
Example of a basic Bicyclic conformation:

Trans-decalin:

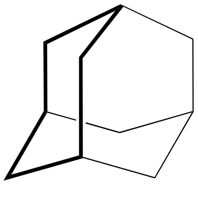


Cis-decalin:





Norbornane



Adamantane

Reactions of alkanes: two will be considered

Further reading: Wade, L.G. Jr., *Organic Chemistry; Custom Edition for the University of Alberta, Chemistry 164/261*, Volume 1, Pearson Learning Solutions, Canada. Pp 176-181

1) **Combustion – already discussed**

$$\text{R-H} + O_2 \xrightarrow{\textbf{heat}} CO_2 + H_2O$$

R=Any alkyl group

2) **Halogenation of alkanes**

$$\text{R-H} + X_2 \xrightarrow{\text{Light } (h\upsilon)} \text{R-X} + \text{HX}$$

R= any alkane (group), R-X = alkyl halide / haloalkane (X=Cl, Br, F); I_2 fails

Substitution reaction – substitute H with X

eg.

$$CH_4 + Cl_2 \xrightarrow{h\upsilon} CH_3Cl + HCl$$

methane

methyl chloride
chloromethane

light energy, $E = h\upsilon$
h = Planck's constant 6.6×10^{-34} joules-sec
υ = frequency of light

$$CH_3Cl + Cl_2 \xrightarrow{h\upsilon} CH_2Cl_2 + HCl$$

methylene chloride
dichloromethane

$$CH_2Cl_2 + Cl_2 \xrightarrow{h\upsilon} CHCl_3 + HCl$$

chloroform
trichloromethane

$$CHCl_3 + Cl_2 \xrightarrow{h\upsilon} CCl_4 + HCl$$

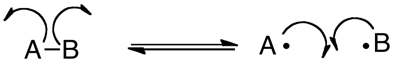
carbon tetrachloride
tetrachloromethane

Mechanism of reaction:

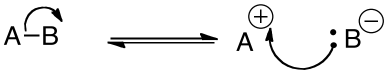
- step by step description of what happens during a reaction (hypothesis)

Two kinds of mechanism-

1. homolytic : (one electron to each atom connected by a bond) radical rxn eg. halogenation of alkanes.



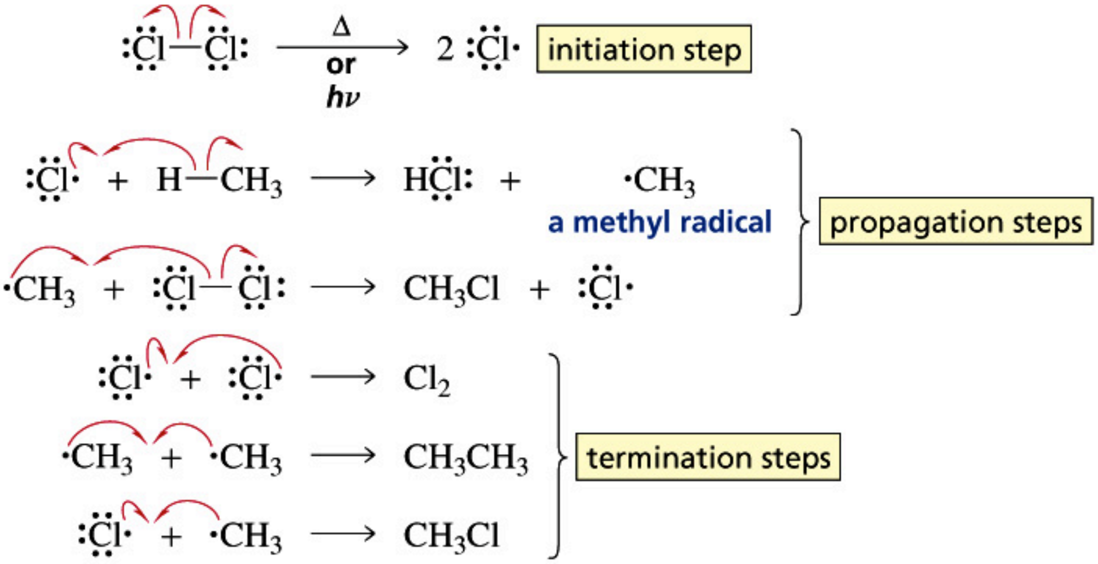
2. heterolytic : (both electrons in bond go to one atom) eg. addition reactions of alkenes, elimination reactions.



Homolytic reactions (less common than heterolytic reactions)
- initiated by heat (Δ) or by light (hυ)

Mechanism of halogenation of CH_4:

$$CH_4 + X_2 \xrightarrow{h\upsilon} CH_3X + HX$$



Note: above mechanism applies to other halogens (F, Cl, Br)