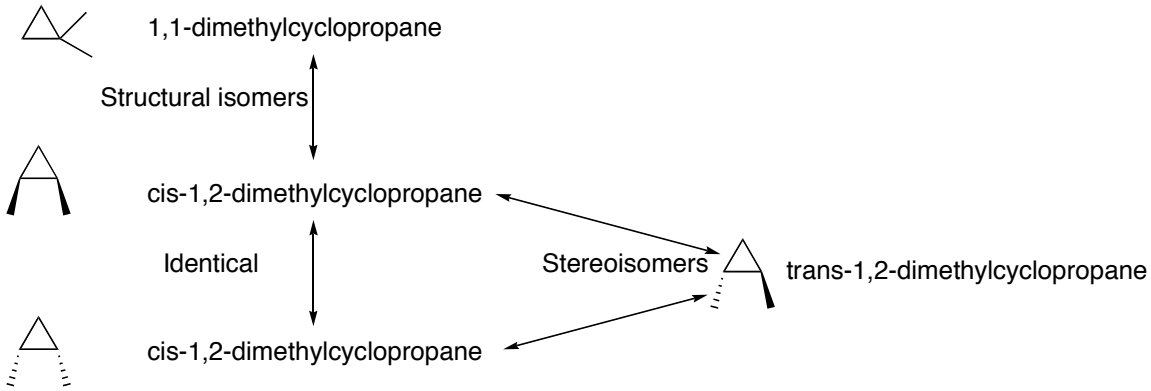
REVIEW:

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

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

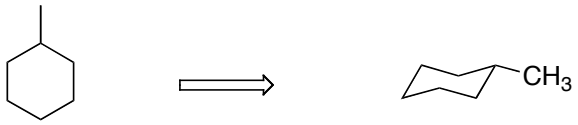
1. structural/constitutional isomers
   – compounds with same molecular formula
2. Stereoisomers – same connectivity but different 3-D structure – 2 sub-types
   (a) diastereomers/diastereoisomers (geometric isomers)
   (b) enantiomers (non-superposable mirror images of same molecule)

eg.

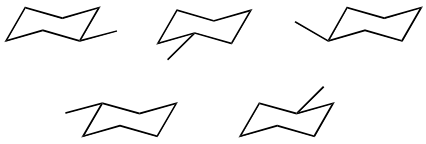


Cyclohexane – conformations

Eg. 1

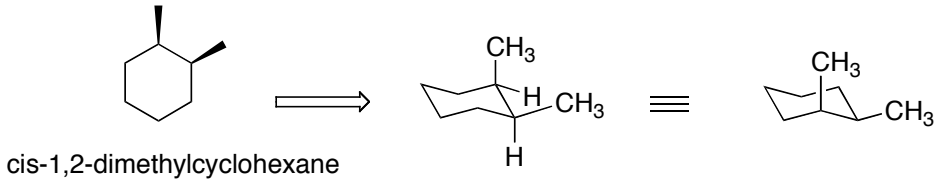


The below are all equally valid representations

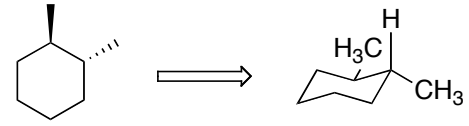


- most stable conformation is when methyl group is equatorial

Eg. 2



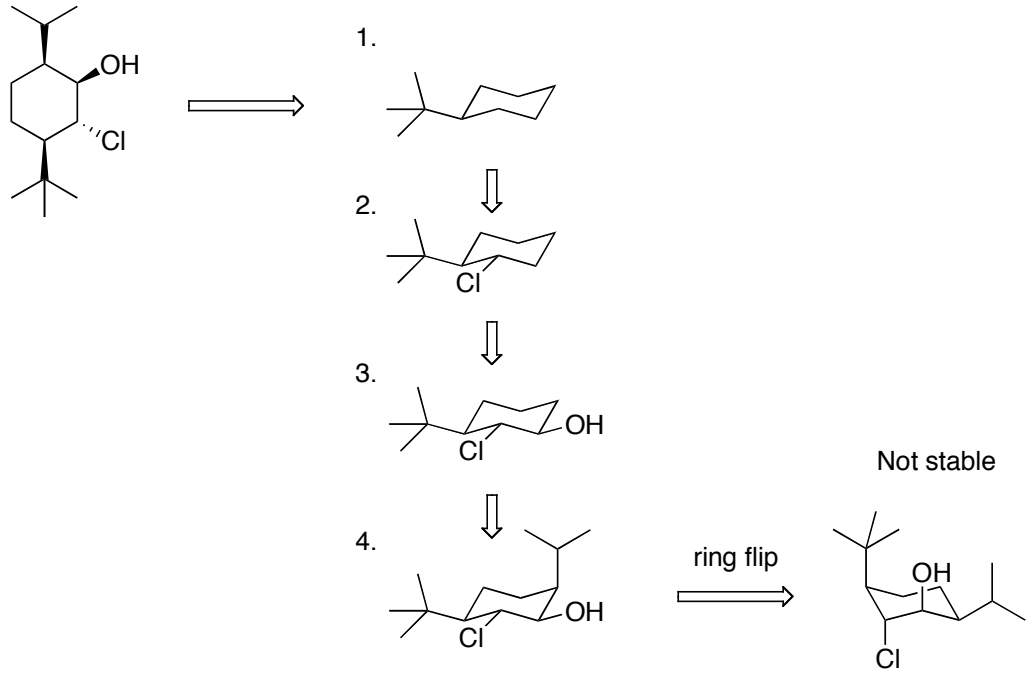
cis-1,2-dimethylcyclohexane



trans-1,2-dimethylcyclohexane

Eg. 3

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

Reactions of alkanes: Two will be considered

1) Combustion – already discussed

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

R=Any alkyl group

2) Halogenation of alkanes

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

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

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

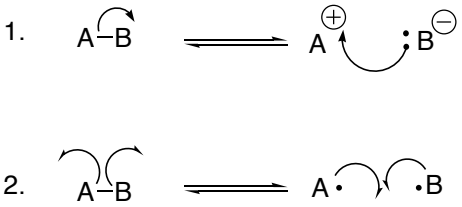
carbon tetrachloride, tetrachloromethane

Mechanism of reaction:

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

Two kinds of mechanism-

1. heterolytic : (both electrons in bond go to one atom)
2. homolytic : (one electron to each atom connected by a bond) radical rxn

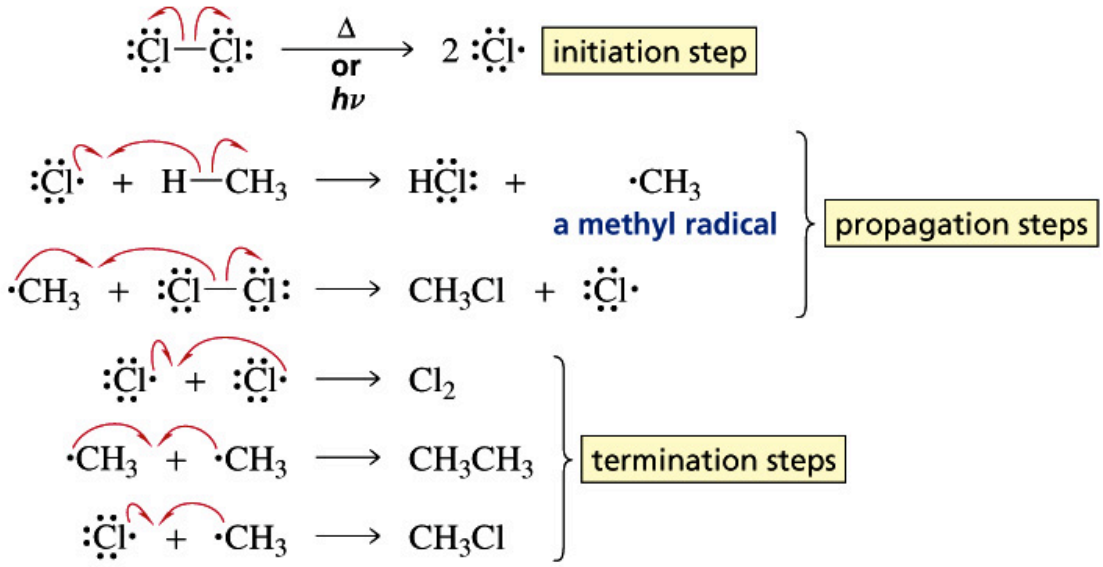


Homolytic reactions (rarer than heterolytic reactions)
- initiated by heat (Δ) or by light (hυ)

Mechanism of halogenation of CH_4:

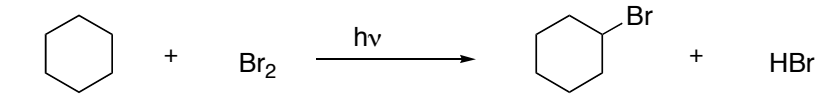
$$CH_4 + X_2 \xrightarrow{h\upsilon} CH_3X + HX$$

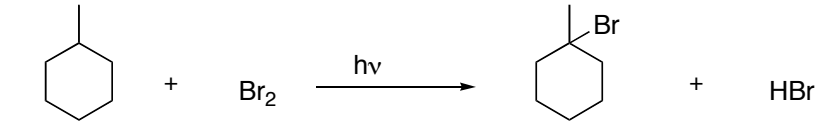
X = F, Cl, Br

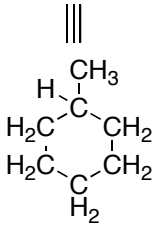


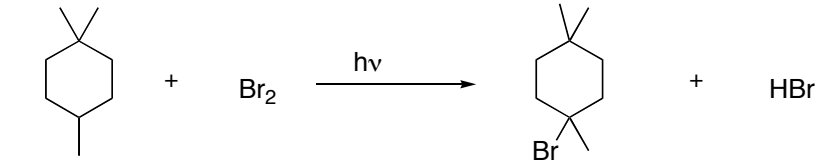
Note: above mechanism applies to other halogens (F, Cl, Br)

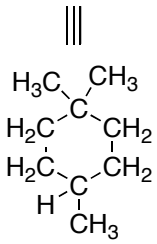
Further examples -

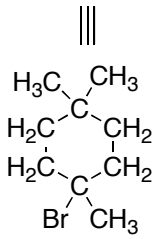
A. 

B. 



C. 





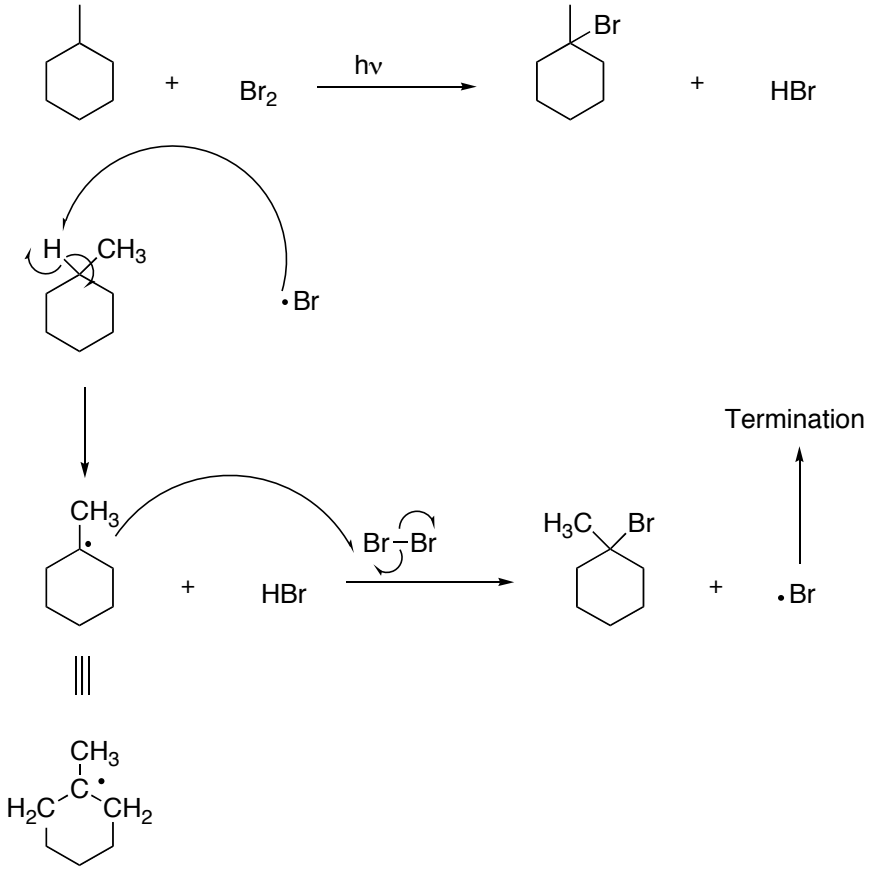
Stability of radicals:

Increases with alkyl substitution.
Alkyl groups are polarizable and donate electrons to electron deficient sites.

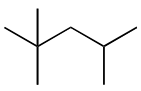
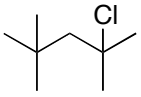
$\cdot CH_3$	<	$\cdot CH_2R$	<	$\cdot CHR_2$	<	$\cdot CR_3$
methyl radical (least stable)		primary radical		secondary radical		tertiary radical (most stable)

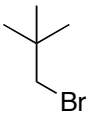
eg.

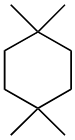
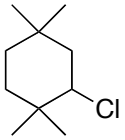
Detailed mechanism



Further Examples

1.  + Cl_2 $\xrightarrow{h\nu}$  + HCl

2.  + Br_2 $\xrightarrow{h\nu}$  + HBr

3.  + Cl_2 $\xrightarrow{h\nu}$  + HCl