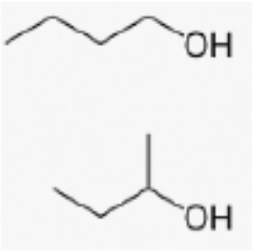
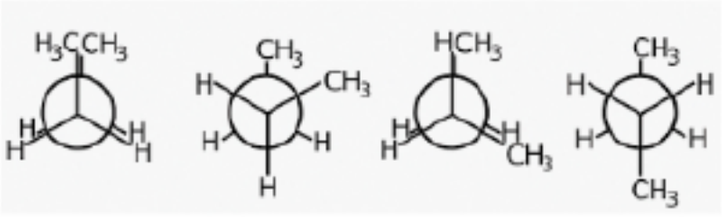
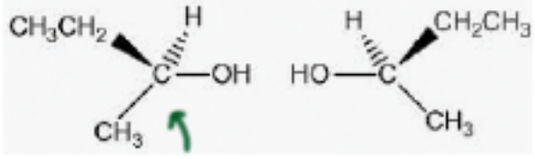
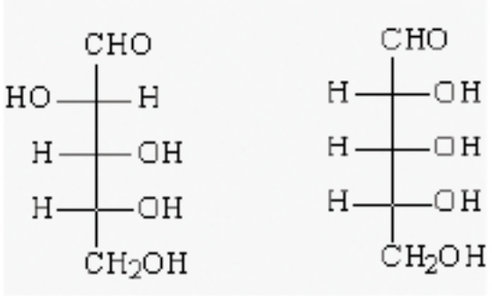
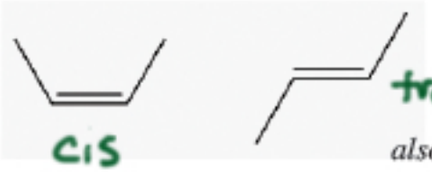
Module 2

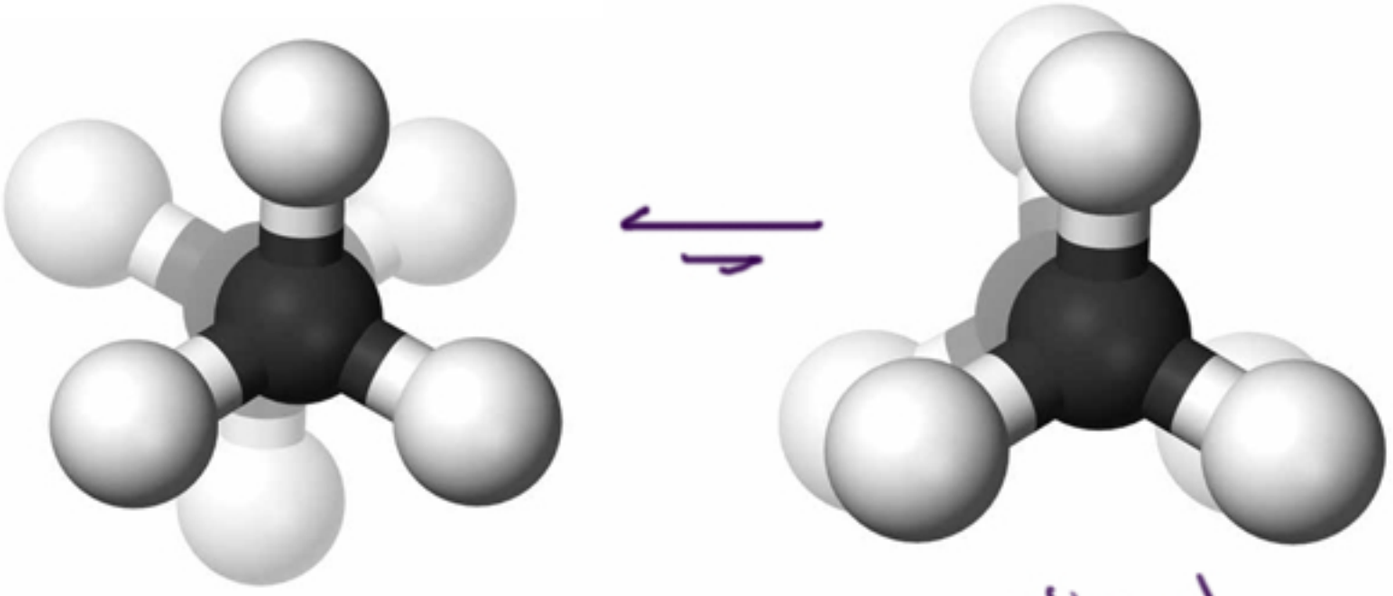
Stereochemistry

Session Slides with Notes

Stereoisomerism

- Isomers
  - different connectivity
    - Constitutional
      - tautomers - constitutional isomers that interconvert
      
    - Stereoisomers
      - Conformational
        
        conformations of butane
      - Optical
        - Enantiomers
          
          chiral center
          non superimposable mirror images
        - Diastereomers
          
      - Geometric
        
        cis
        trans
        also technically diastereomers

Conformational isomerism

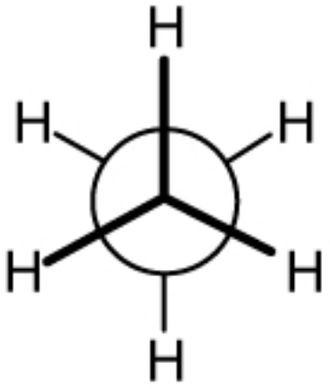


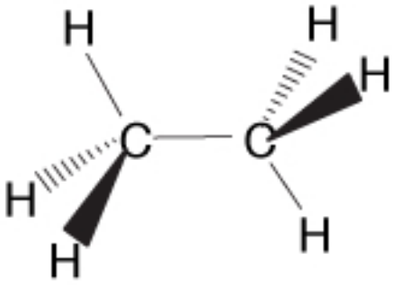
staggered

eclipsed

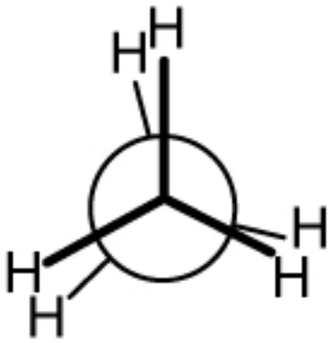
$CH_3\,CH_3$

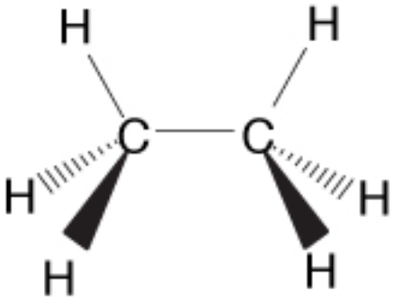
$$K = e^{-\Delta G^{\circ}/RT}$$



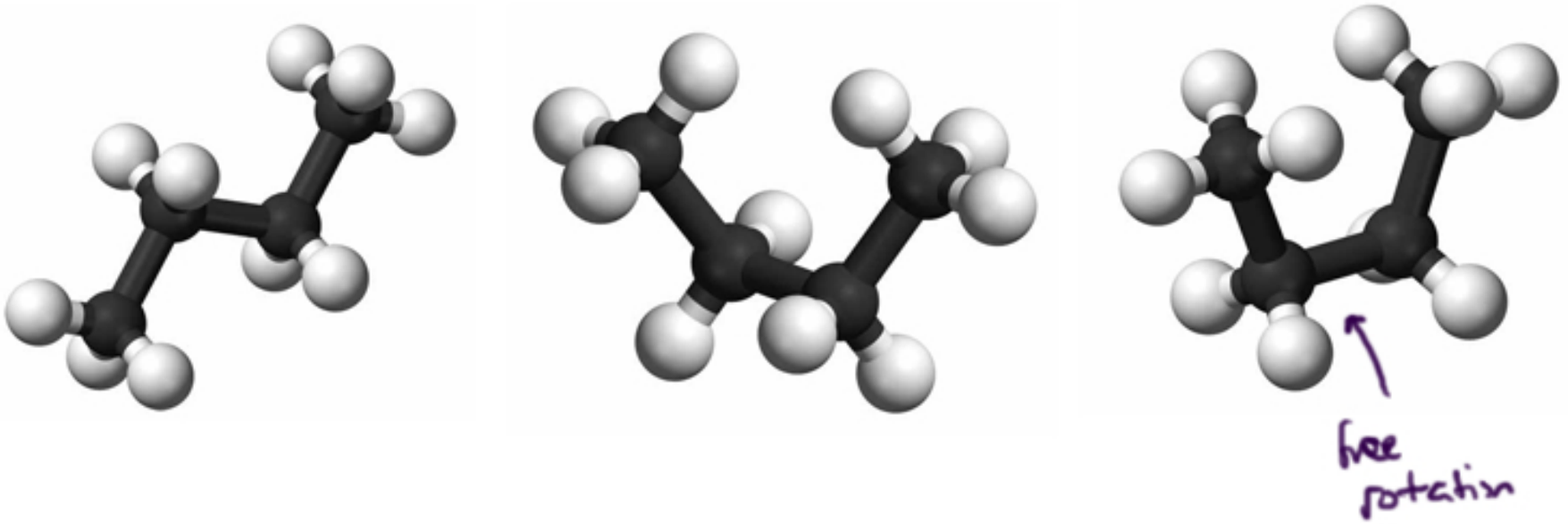


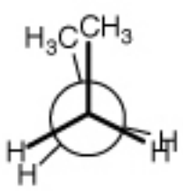
conformations of ethane

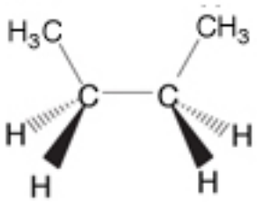




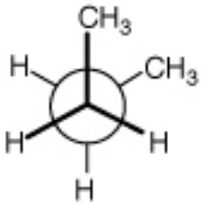
Conformations of butane

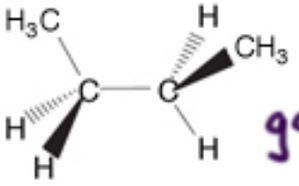




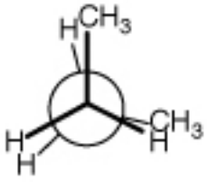


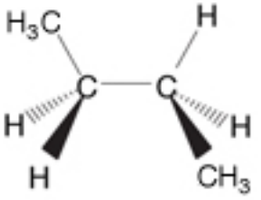
methyl eclipsed



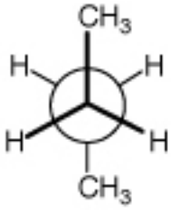


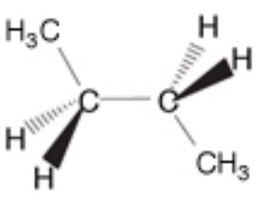
gauche



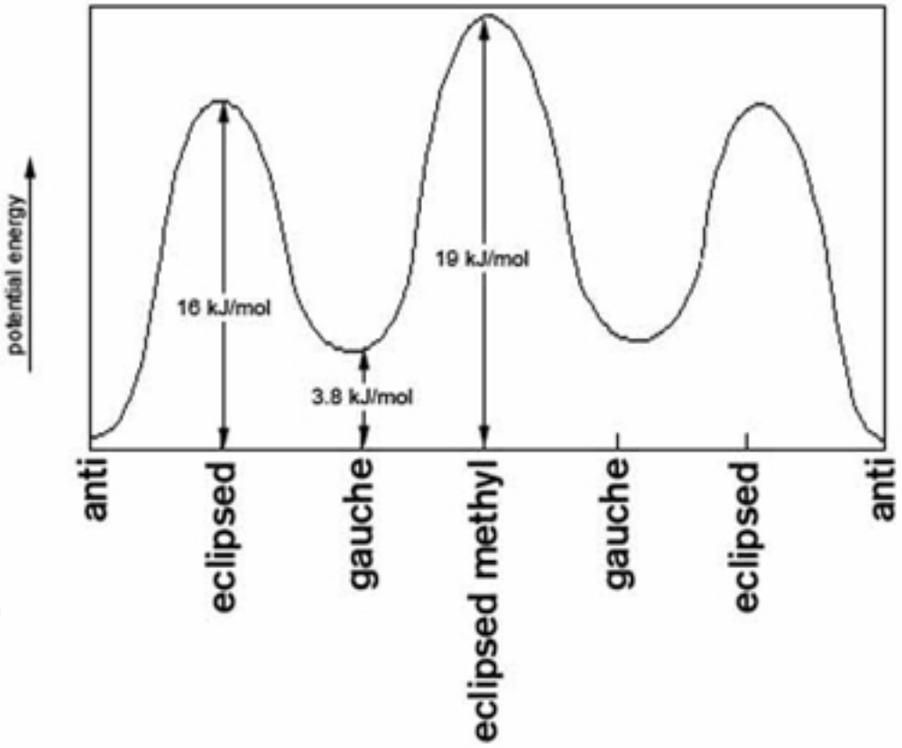


eclipsed





anti



eclipsed methyl $\longrightarrow$ anti

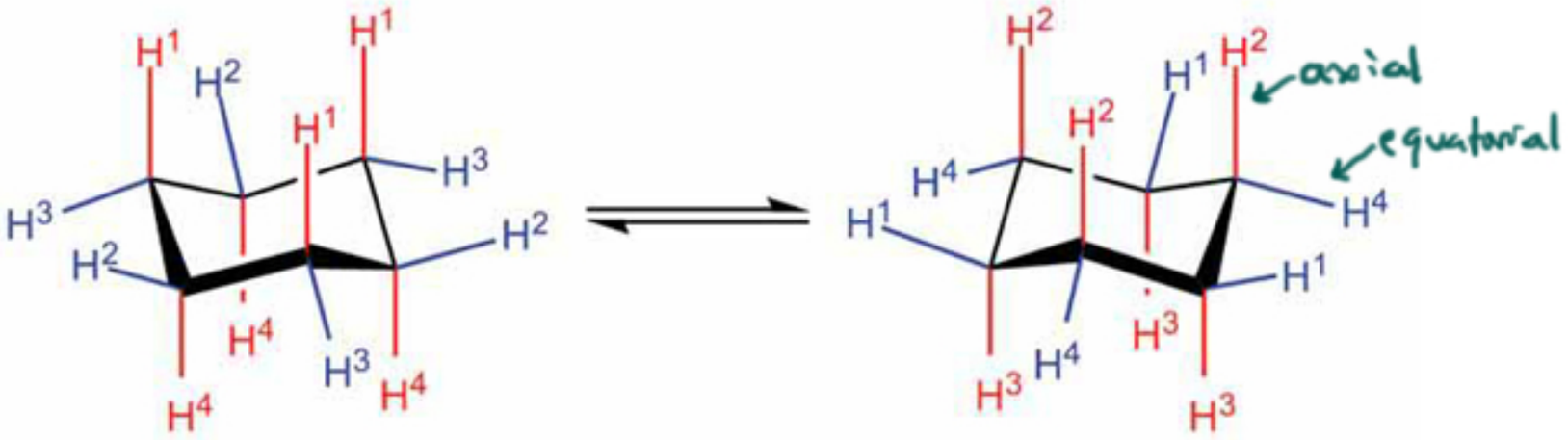
$\Delta G^\circ = -20\ kJ/mol$

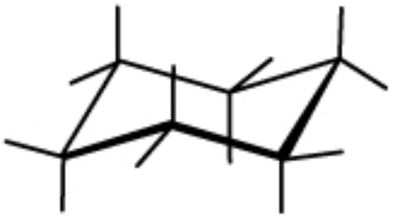
$K = \frac{[B]}{[A]}$ $K = e^{-\Delta G^\circ/RT}$

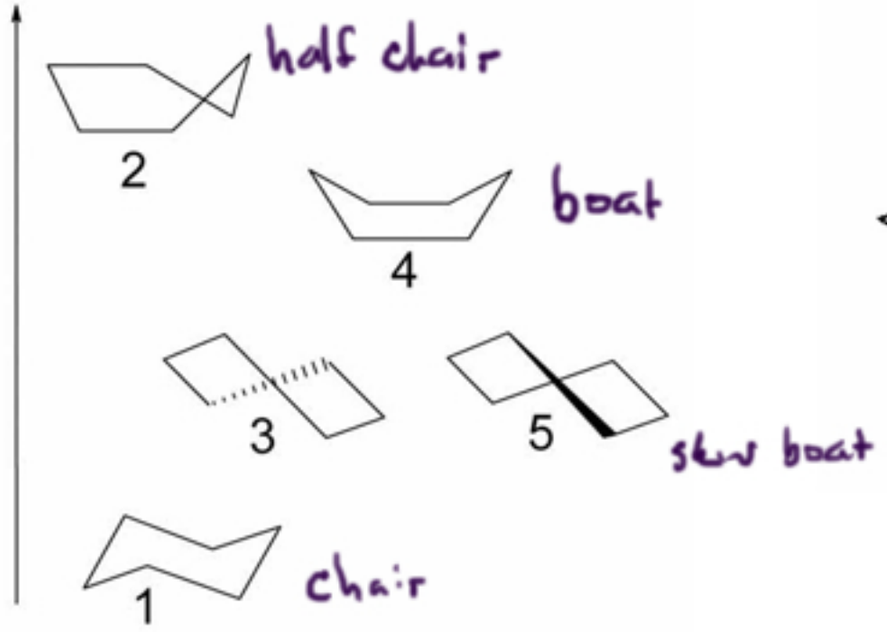
$K = e^{+20{,}000/(8)(300)}$

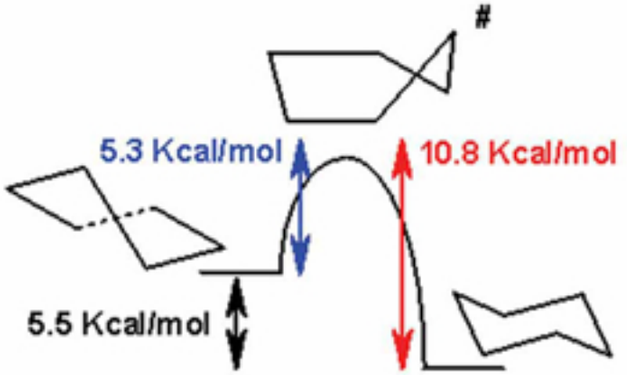
$\sim e^{8} \sim 500$

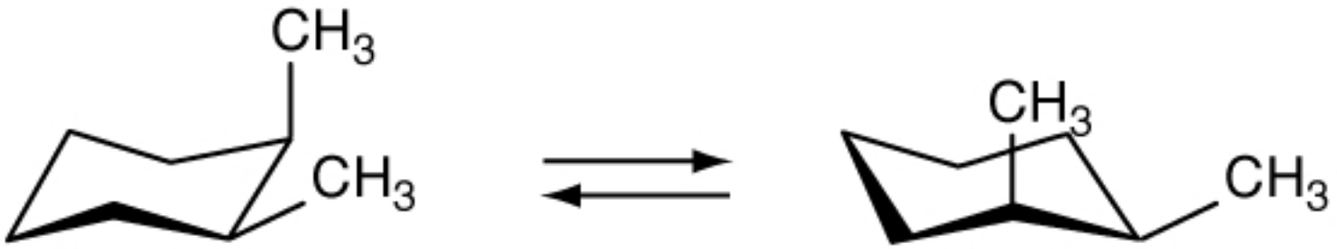
Ring flipping in cyclohexane

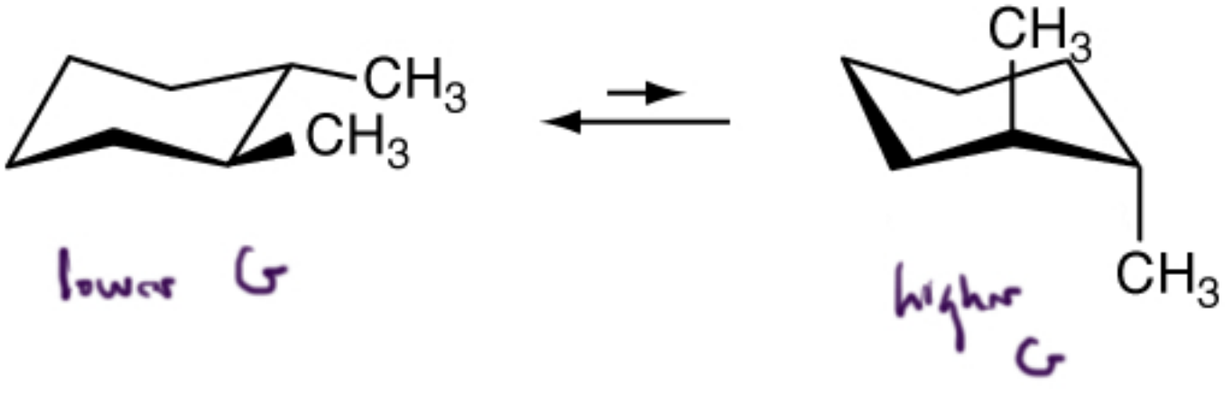


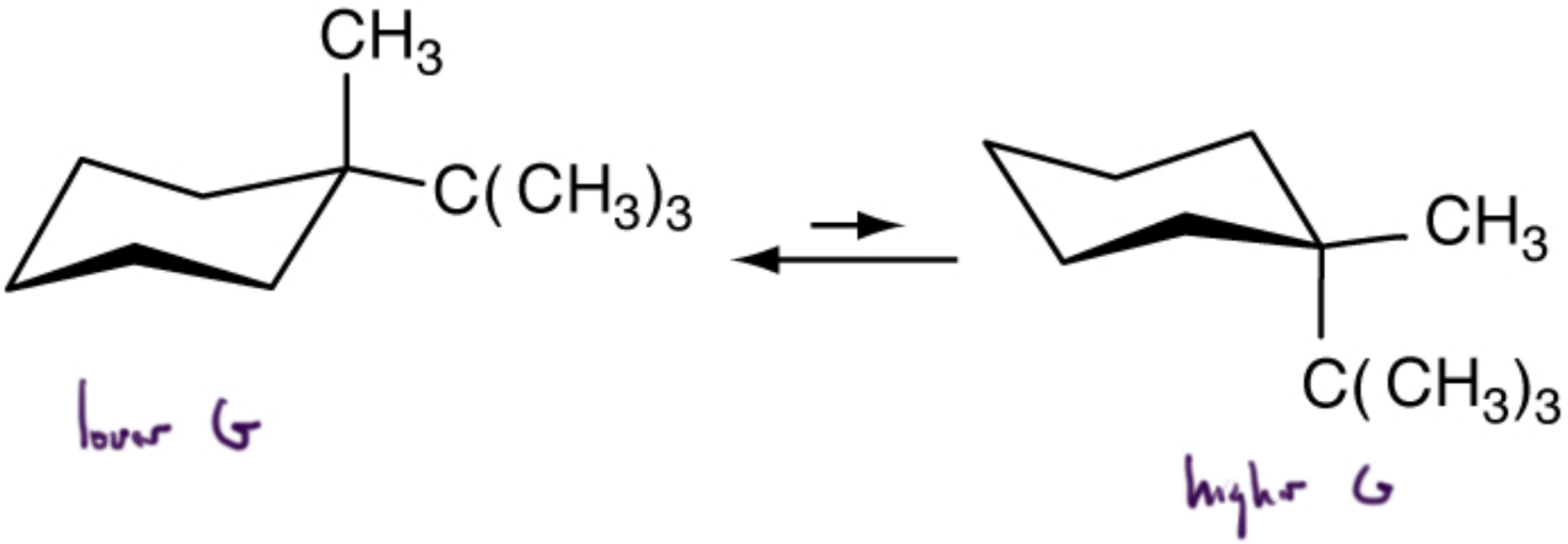



half chair
2
boat
4
3
5
skew boat
1
chair


#
5.3 Kcal/mol
10.8 Kcal/mol
5.5 Kcal/mol

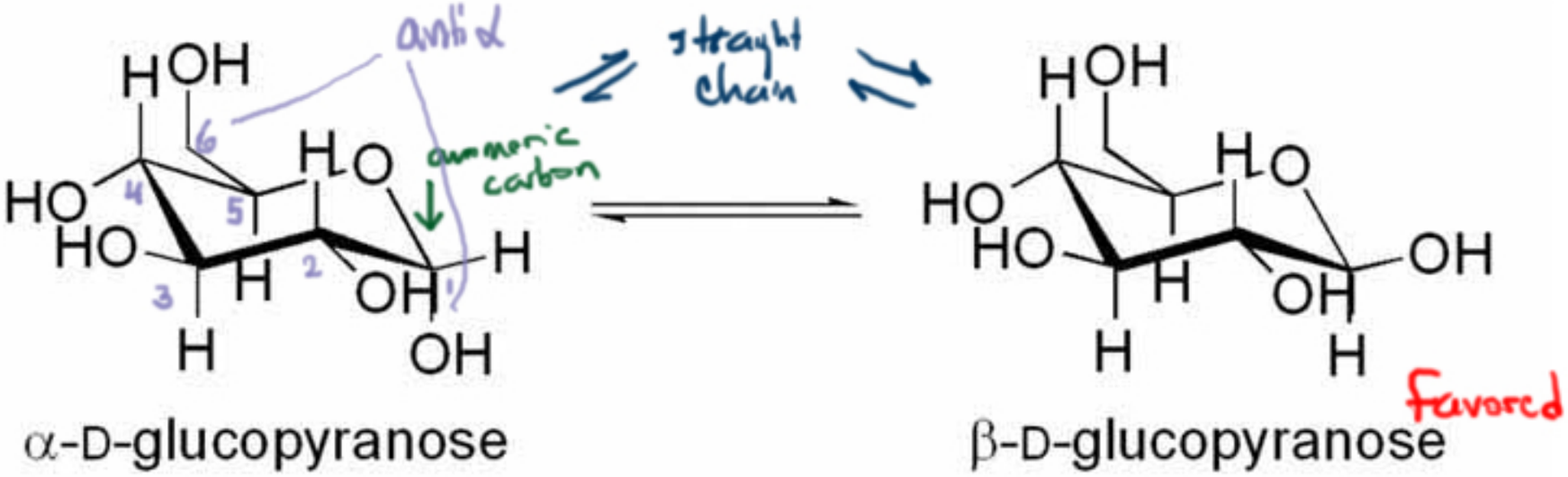

CH3
CH3
CH3
CH3


CH3
CH3
CH3
CH3
lower G
higher G



lower G

higher G

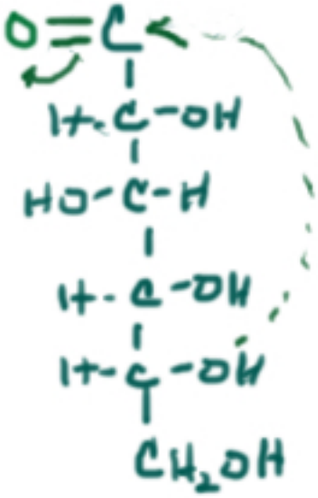


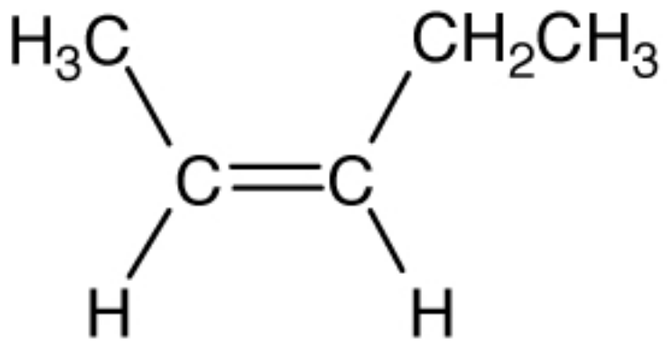
α-D-glucopyranose

β-D-glucopyranose

Pyranose means 6 membered ring

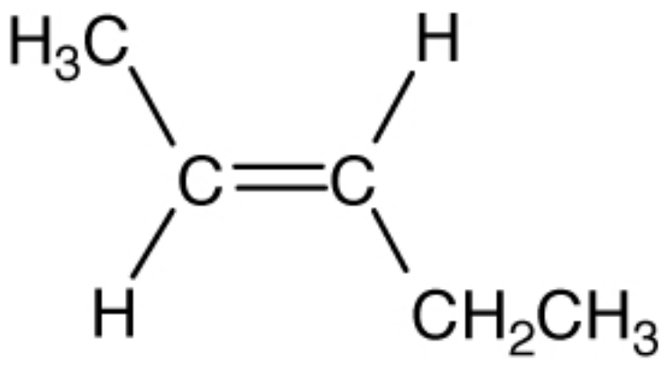
same as β-D-glucose





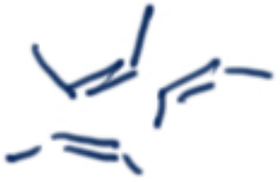
higher G

cis



trans

higher melting point

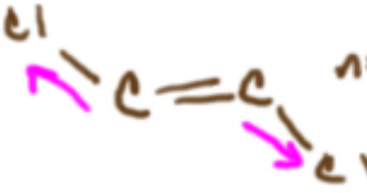


more access for van der Waals

However

dipole dipole

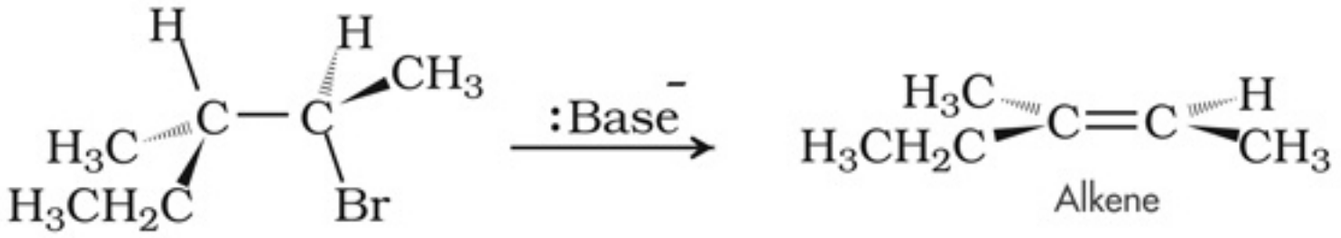
higher melting



no net dipole moment

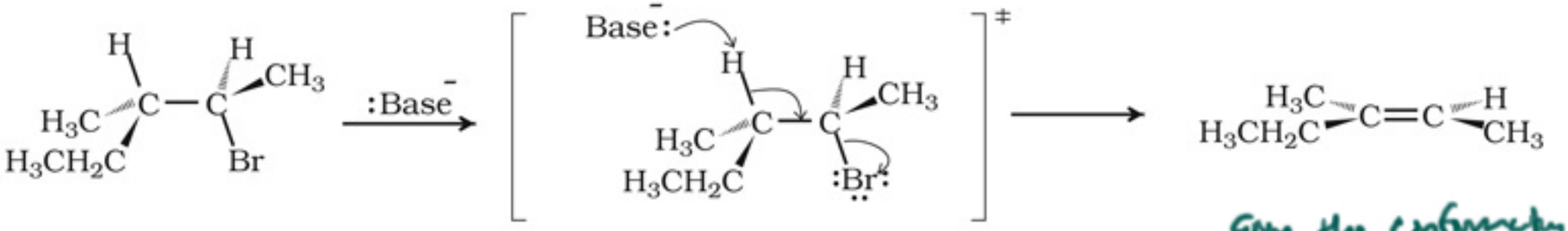
only Van der Waals

E2



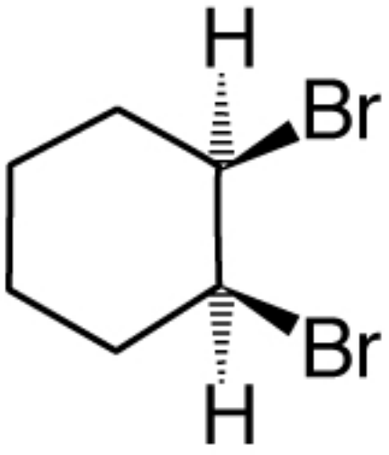
Alkyl halide

Alkene

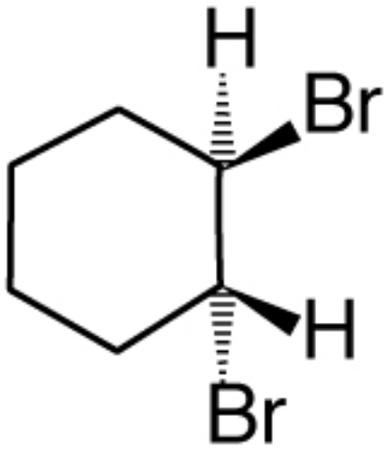


anti periplanar transition state

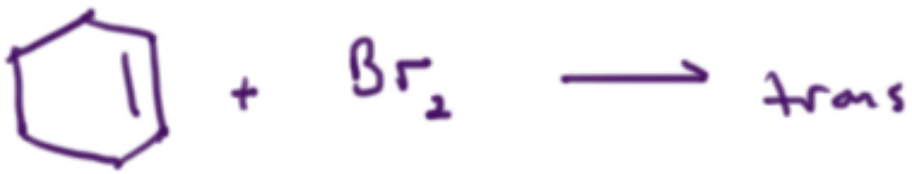
Given the conformation of the reagent, this reaction is stereospecific for cis product



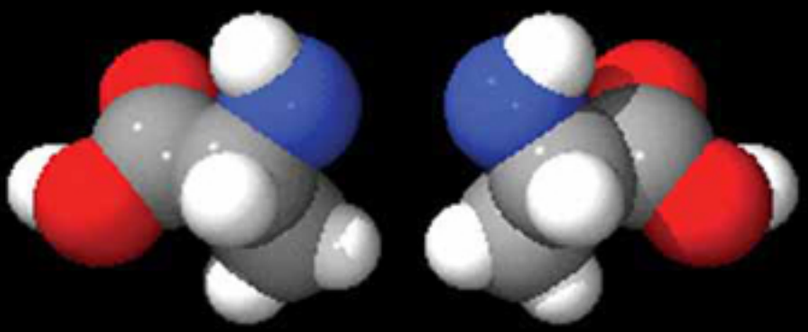
cis



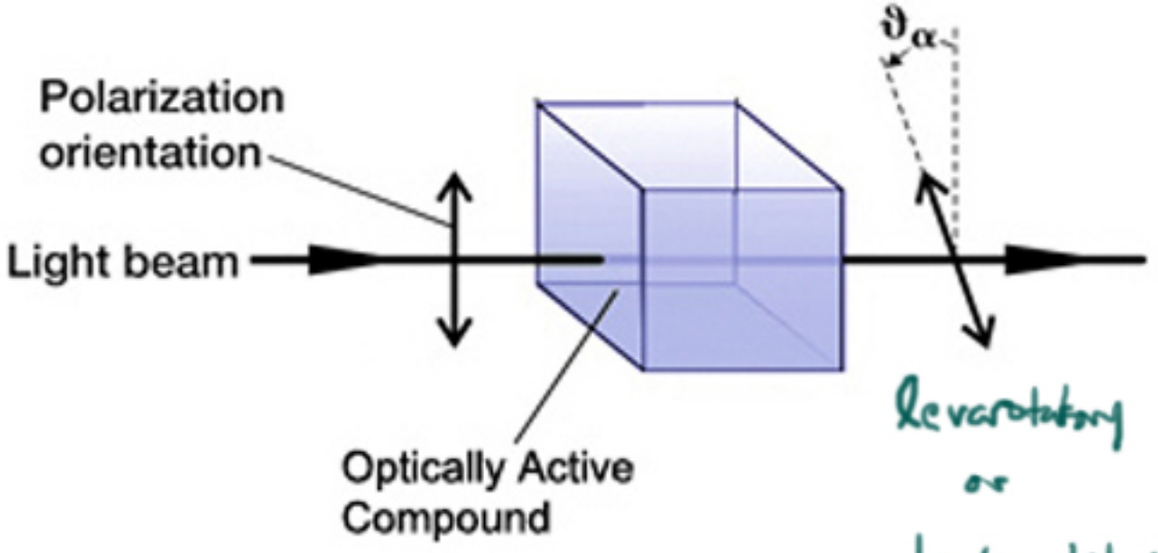
trans



optical isomers



enantiomers
mirror images



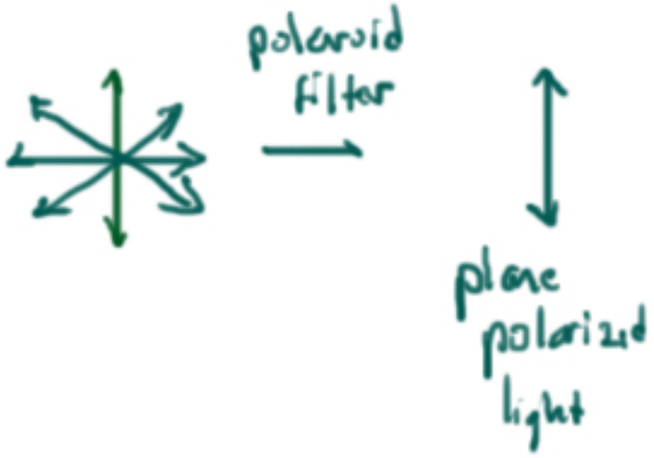
specific rotation → $[\alpha]_\lambda^T = \frac{\alpha}{l \times \rho}$ ← observed rotation

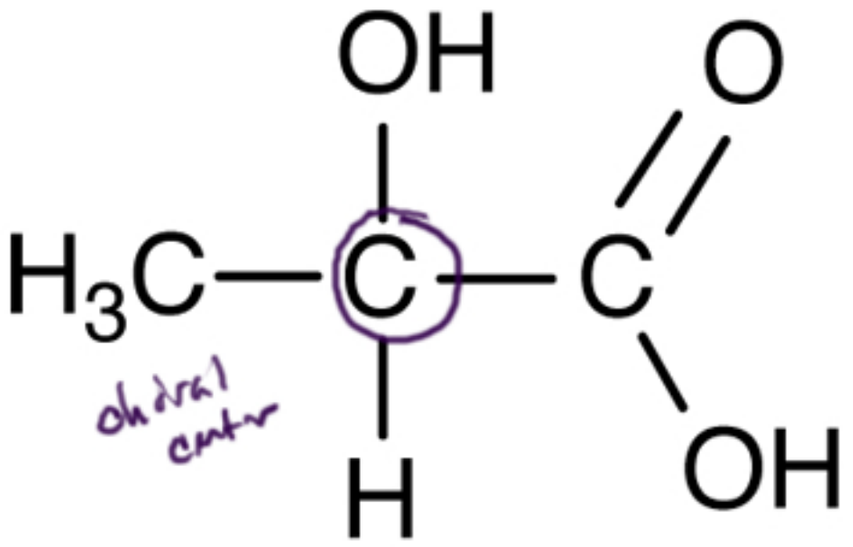
path length ↑ ↑ concentration

levorotatory or dextrorotatory

an optical isomer may be d or l

(THIS IS NOT THE SAME AS D and L)

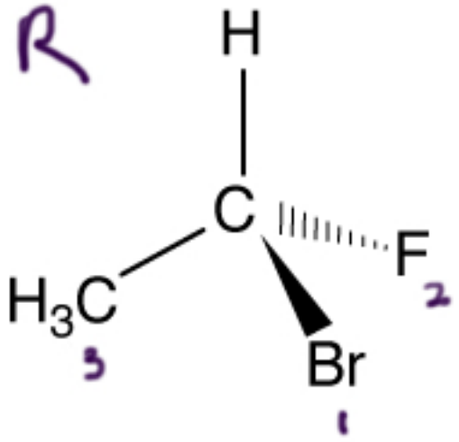


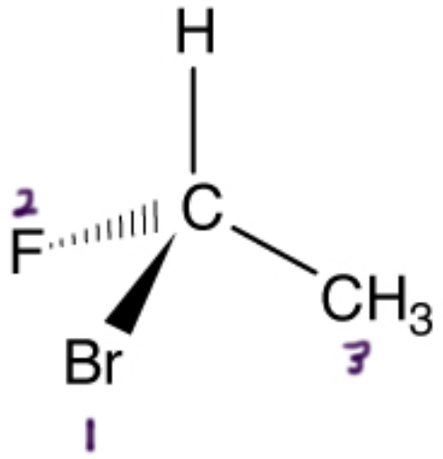


Lactic Acid

Two Enantiomers

R



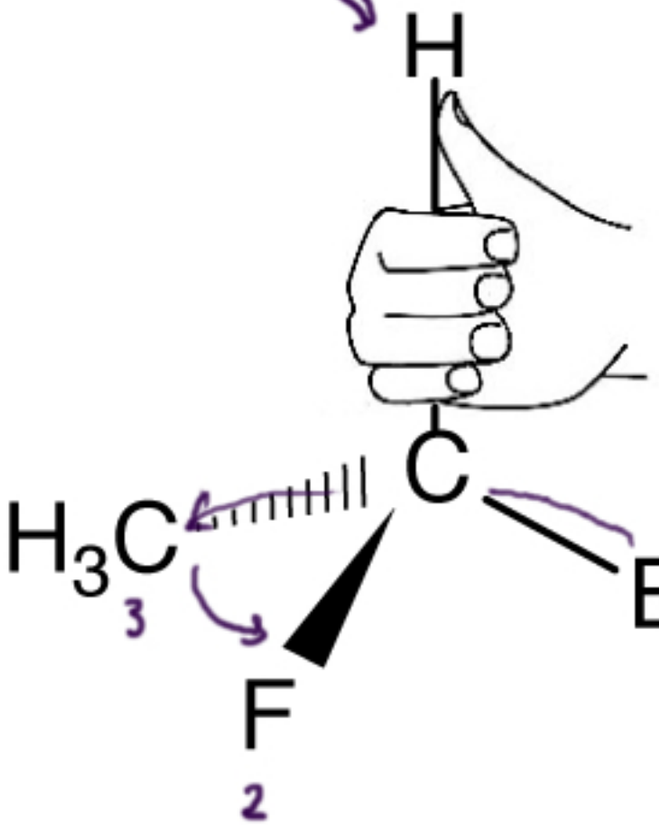


S

1 ⇒ 2 ⇒ 3

lowest rank

Cahn Ingold Prelog System



1 ⇒ 3 ⇒ 2

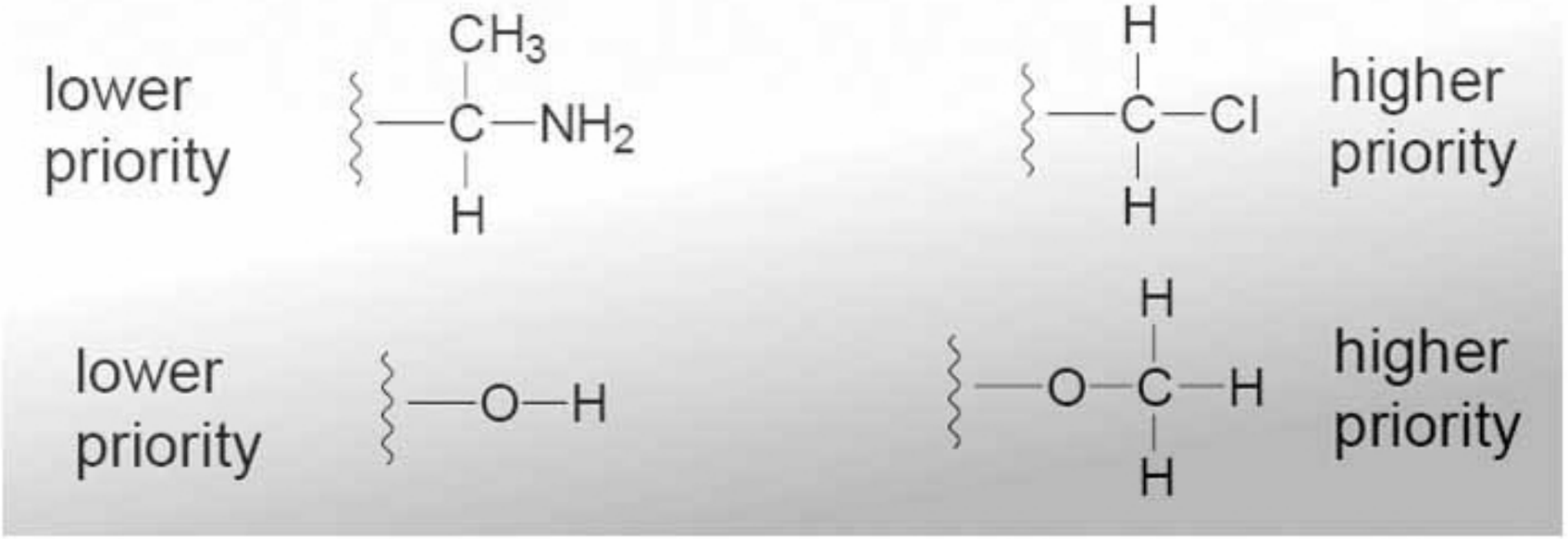
that's S

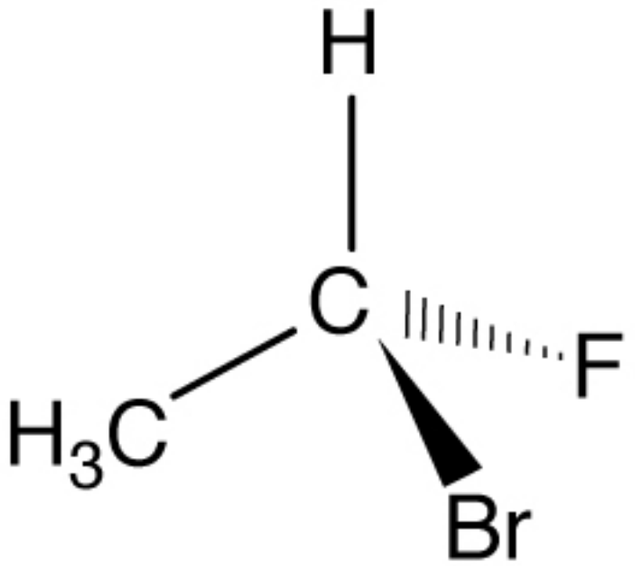
if it had been

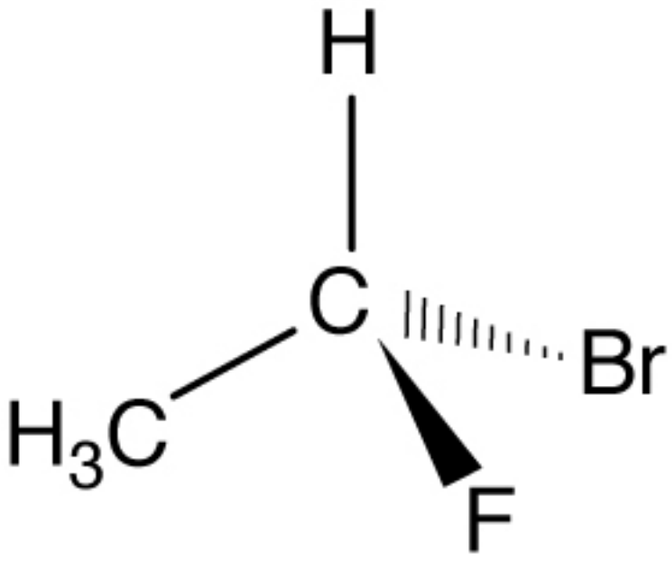
1 ⇒ 2 ⇒ 3

that's R

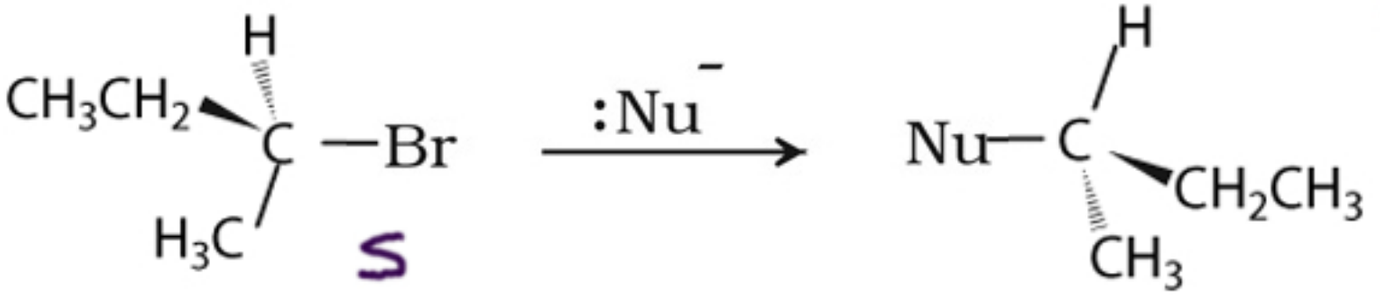
Practice!


lower priority
CH3
C
NH2
H
H
C
Cl
H
higher priority
lower priority
O
H
H
O
C
H
H
higher priority


H
C
F
H3C
Br

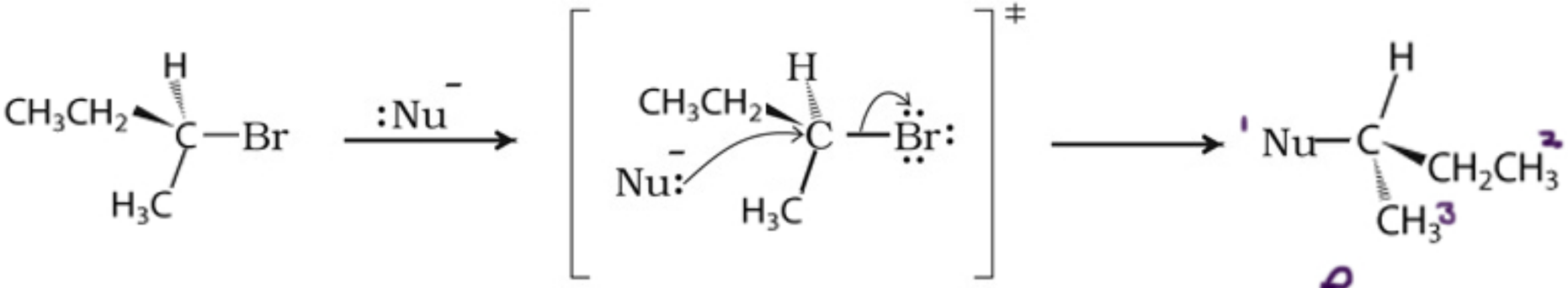

H
C
Br
H3C
F

SN2



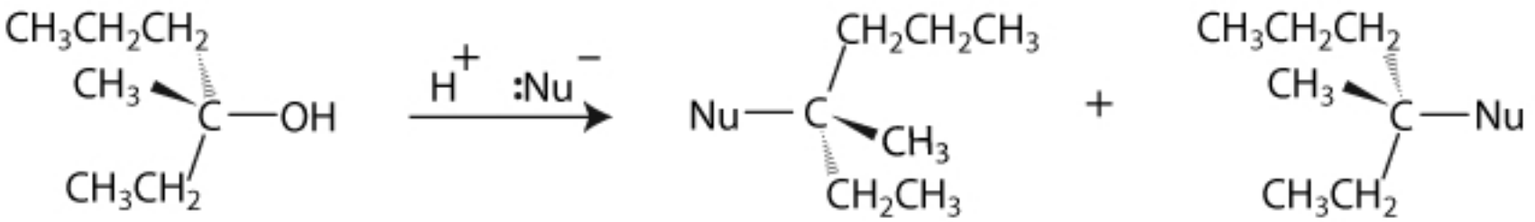
Alkyl halide

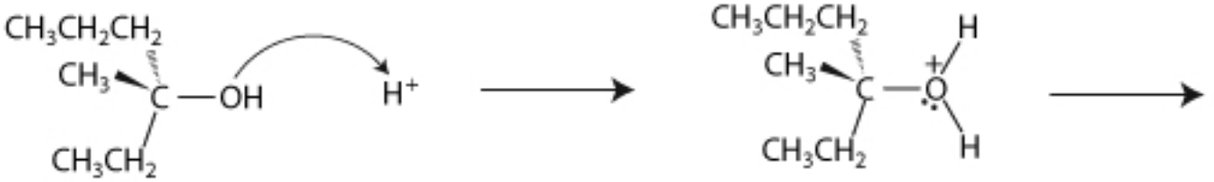
Substitution product

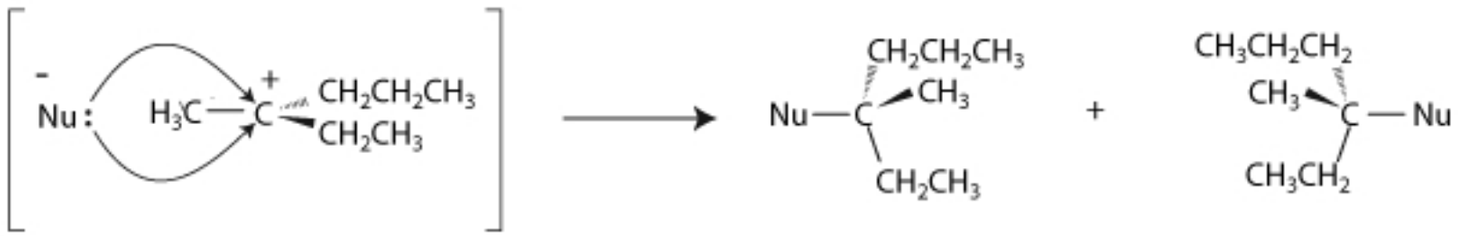


stereospecific for
inversion of configuration

SN1 Substitution



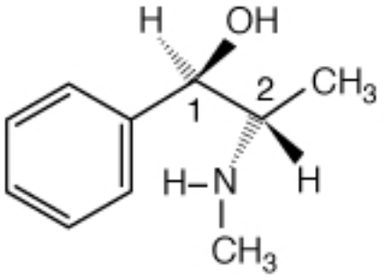




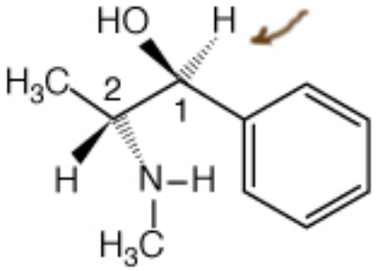
proceeds with racemization

not optically active racemic mixture

diastereomers

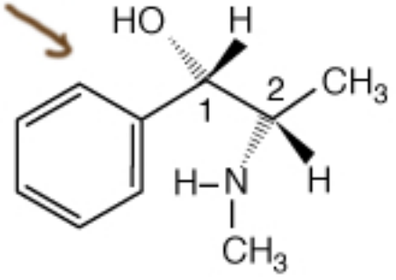


1-(*R*),2-(*S*)

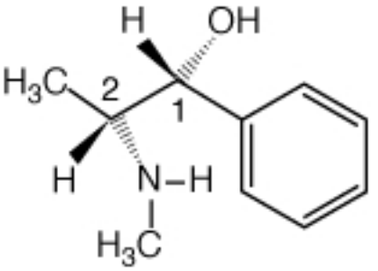


1-(*S*),2-(*R*)

Ephedrine enantiomers



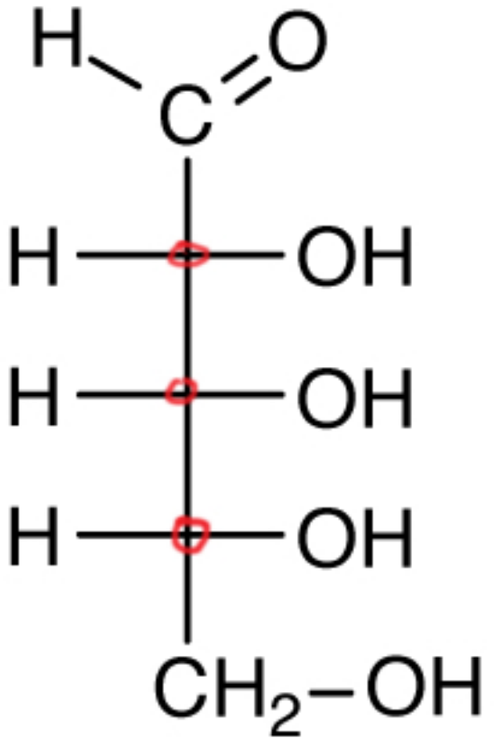
1-(*S*),2-(*S*)



1-(*R*),2-(*R*)

Pseudoephedrine enantiomers

Ribose

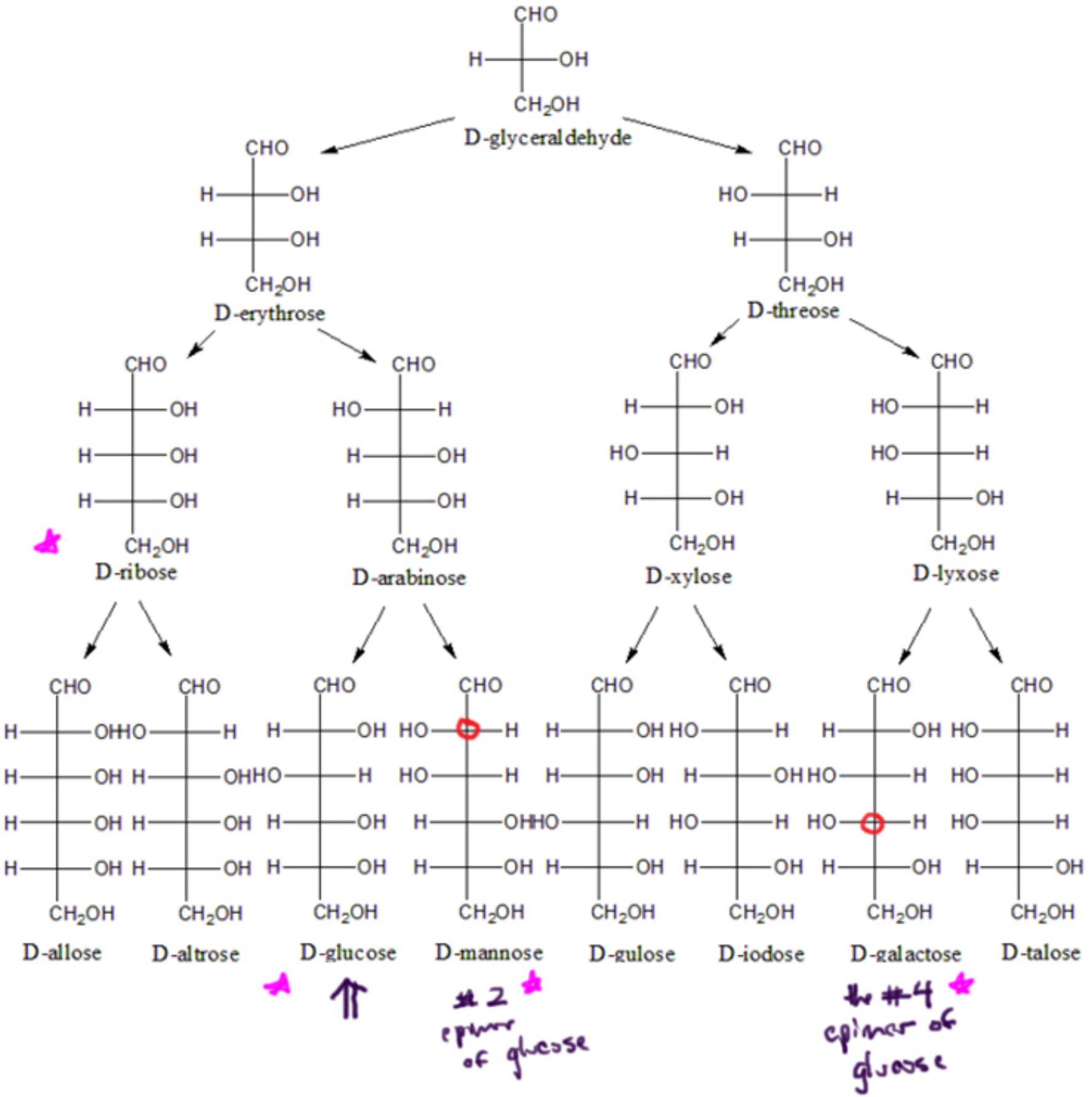


Ribose is one of

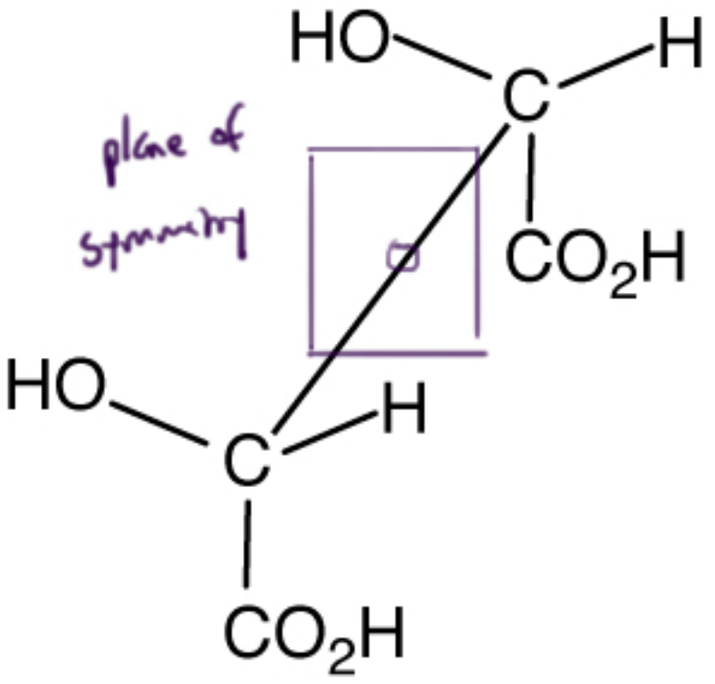
$2^3 = 8$

Stereoisomers

Fischer Projection of D- Aldoses.



Meso Compound



plane of symmetry

actually achiral

not optically active