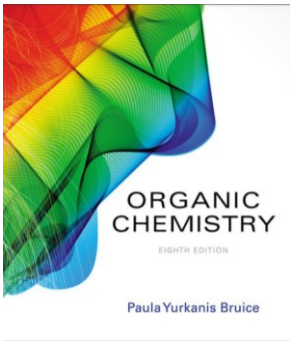
FLORIDA SOUTHWESTERN STATE COLLEGE

CHM 2210

Lecture 05



Outline

- Isomerism
  - Types
    - Cis-Trans
    - R & S
  - Nomenclature

Ch 4 & 13

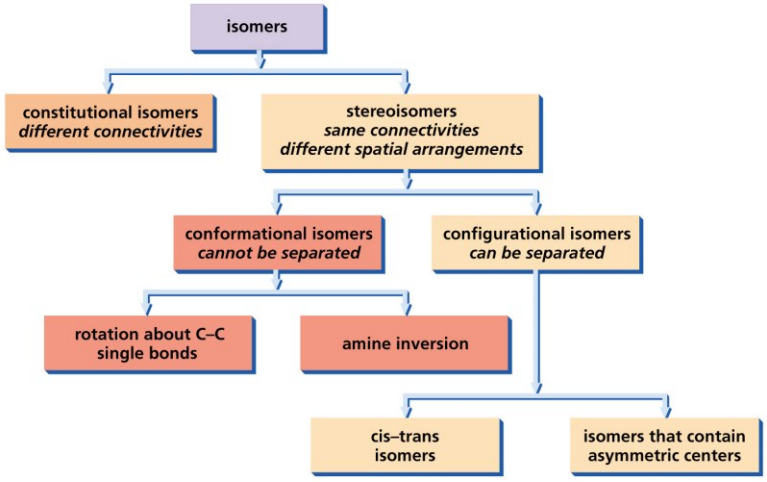
Soumya (SAM) Bhattacharya

1

FLORIDA SOUTHWESTERN STATE COLLEGE

Isomers

- Isomers are compounds that have the same molecular formula but different structures.

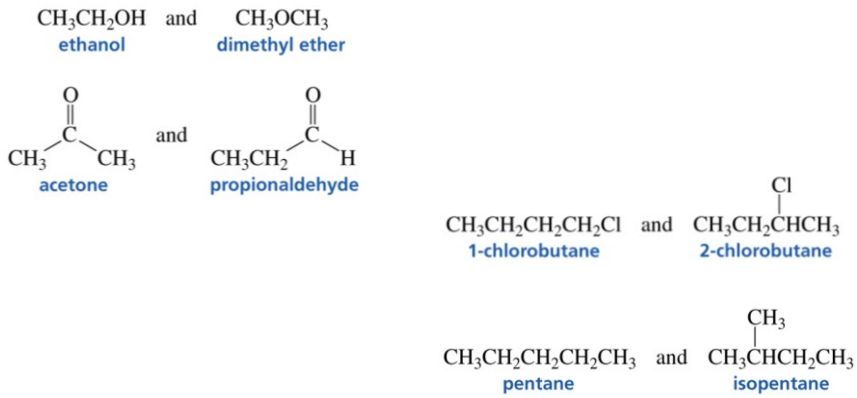


2

2

Constitutional Isomers

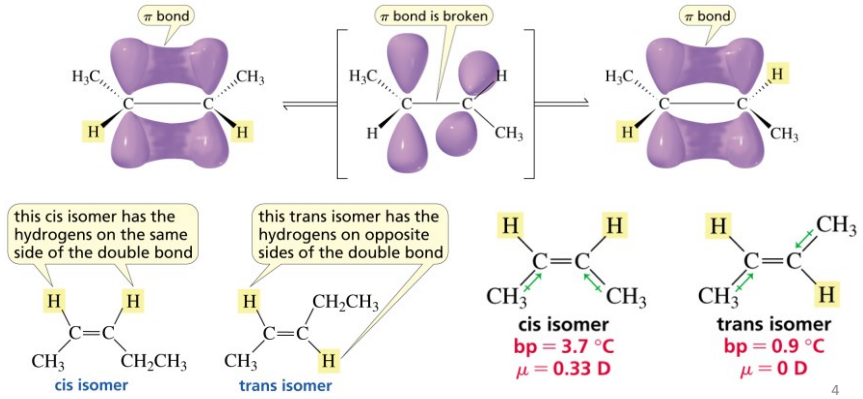
- Constitutional isomers: differ in the way the atoms are connected.



3

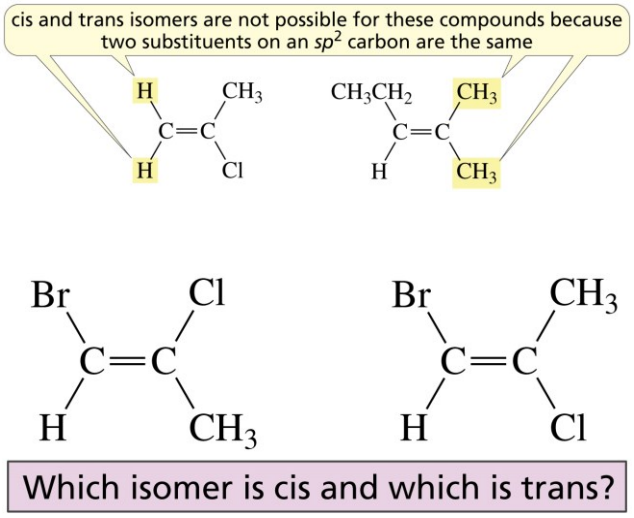
(Z) Cis & (E) $Trans$ Isomerism in Alkenes – I

- Cyclic structures restrict rotation resulting in cis – $trans$ isomer.
  - ✓ Cis: The hydrogens are on the same side of the double bond.
  - ✓ $Trans$: The hydrogens are on opposite sides of the double bond.
- Cis – $trans$ isomers have different physical properties.



4

(*Z*) *Cis* & (*E*) *Trans* Isomerism in Alkenes – II

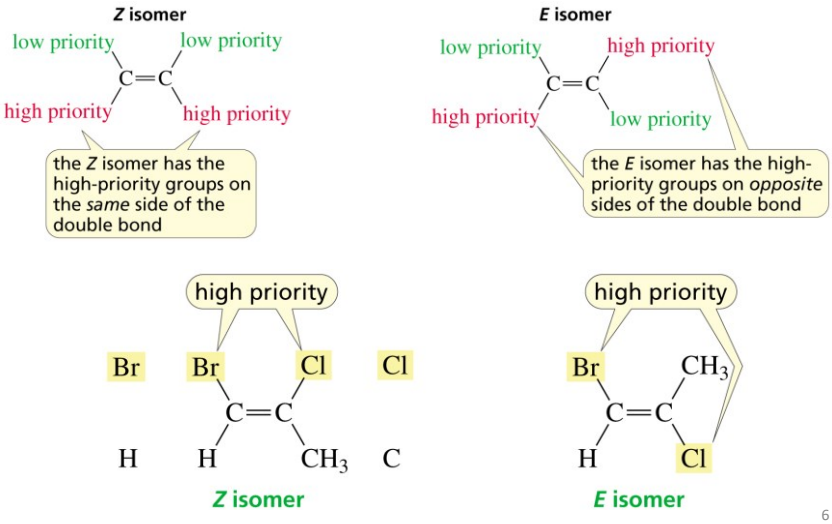


5

(*Z*) *Cis* & (*E*) *Trans* Isomerism in Alkenes – III

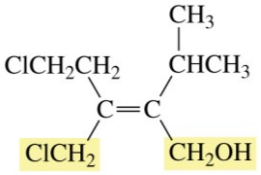
Z = Zusammen (together)

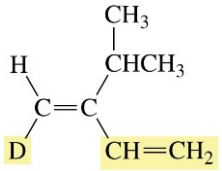
E = Entgegen (opposite)



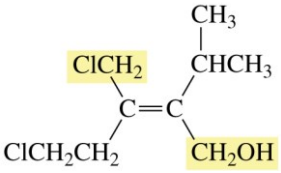
6

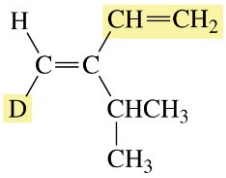
Examples – I





Z - isomer



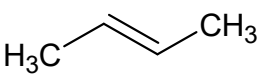


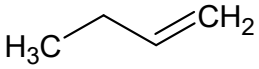
E - isomer

7

7

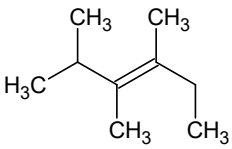
Examples – II

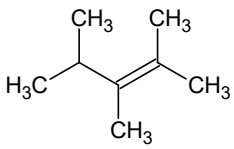




isomeric relationship:

isomeric relationship:

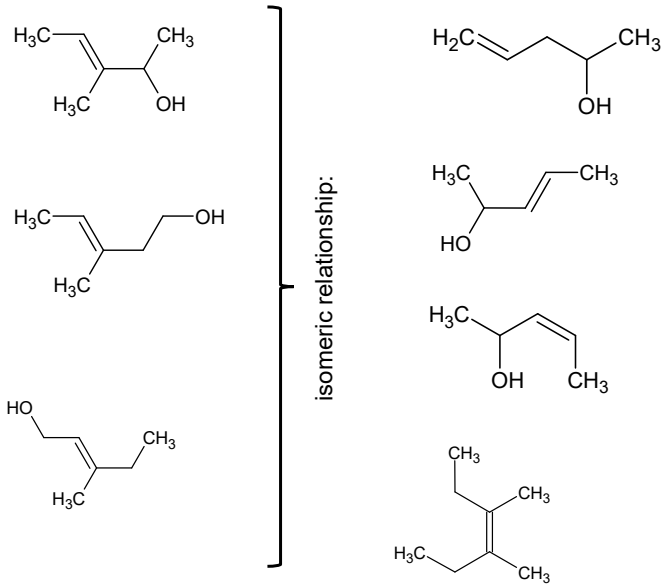




8

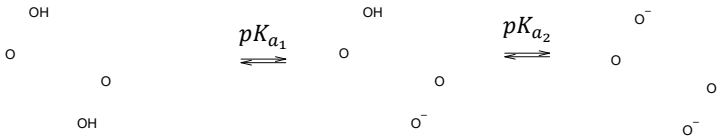
8

Examples – III

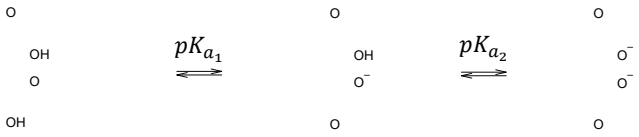


9

(Z) *Cis* & (E) *Trans* Isomerism in Alkenes – IV



Fumaric Acid or $trans$-2-butanedioic acid



Maleic Acid or cis-2-butanedioic acid

$pk_{a_1}(fumaric\ acid) > pk_{a_1}(maleic\ acid)$

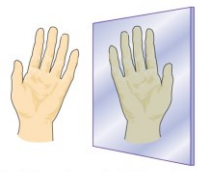
$pk_{a_2}(fumaric\ acid) < pk_{a_2}(maleic\ acid)$

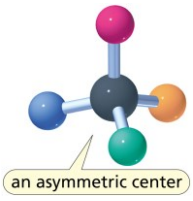
conjugate base stability by H-bond

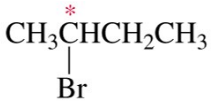
10

Chirality: Alkane Isomerism – I

- A chiral object has a nonsuperimposable mirror image.
- An achiral object has a superimposable mirror image.
- A chiral molecule has an asymmetric center.
- An asymmetric center is an atom that is attached to four different groups.





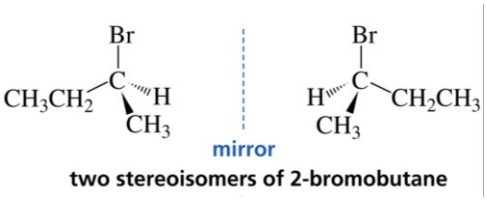


2-bromobutane

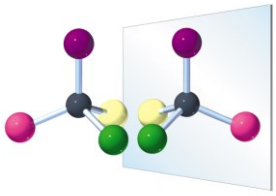
11

Chirality: Alkane Isomerism – II

- The two stereoisomers are called enantiomers.
- Enantiomers are nonsuperimposable mirror images.
- Enantiomers are different compounds: they can be separated.
- Enantiomers have the same physical and chemical properties.



two stereoisomers of 2-bromobutane

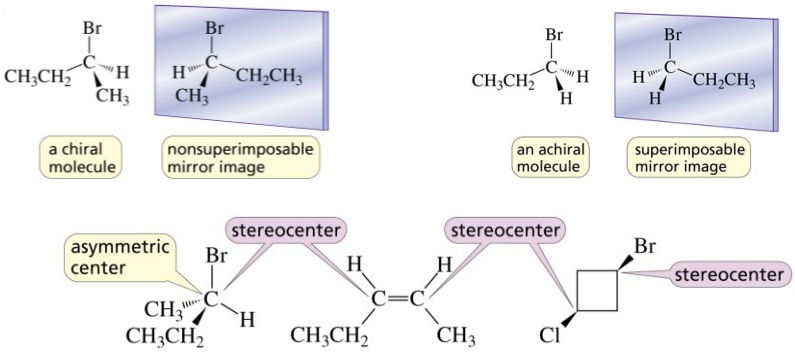


nonsuperimposable mirror images

12

Chirality: Alkane Isomerism – III

- Chiral compound: a nonsuperimposable mirror image MUST exist.
- Achiral compound: no superimposable mirror image exists - identical molecules.
- Asymmetric center: an atom attached to four different groups.
- Stereocenter: an atom at which the interchange of two groups produces a stereoisomer.



13

13

Chirality: Alkane Isomerism – IV

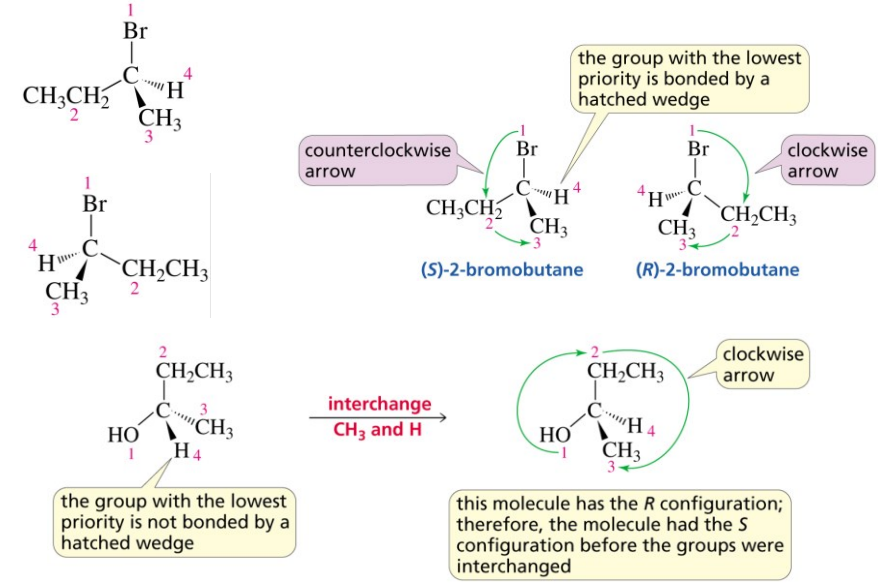
❖ **IUPAC Rules for Prioritization**

- Assign relative priorities to the four groups.
- If the lowest priority group is on a hatched wedge
  - ✓ clockwise = R
  - ✓ counterclockwise = S
- If the lowest priority group is not on a hatched wedge, switch a pair so it is on a hatched wedge.
- If the lowest priority group is on a vertical bond
  - ✓ clockwise = R
  - ✓ counterclockwise = S
- If the lowest priority group is on a horizontal bond
  - ✓ counterclockwise = R
  - ✓ clockwise = S

14

14

Chirality: Alkane Isomerism – V



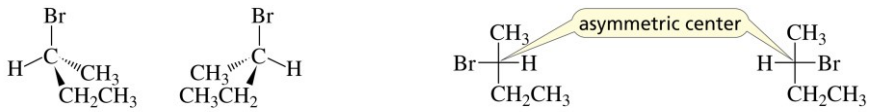
15

15

Chirality: Alkane Isomerism – VI

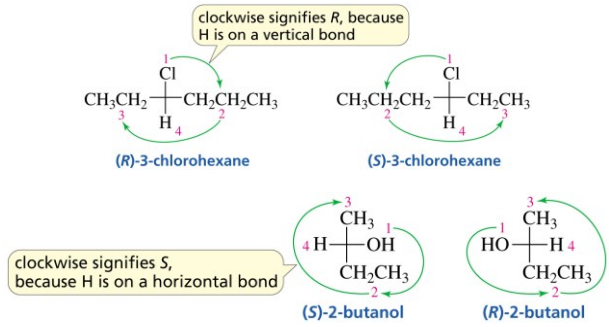
❖ **Perspective Formulas**

❖ **Fischer Projections**



perspective formulas of the enantiomers of 2-bromobutane

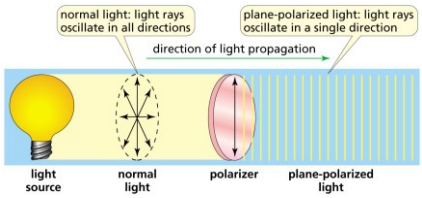
Fischer projections of the enantiomers of 2-bromobutane

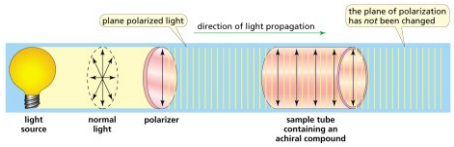


16

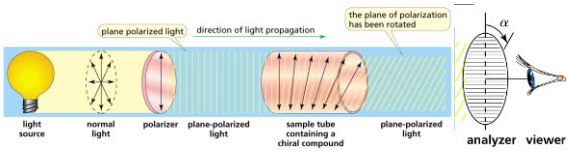
16

Chirality: Alkane Isomerism – VII





$$[\alpha]_{\lambda}^{T} = \frac{\alpha}{l \times c}$$

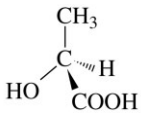


17

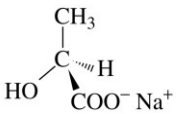
17

Chirality: Alkane Isomerism – VIII

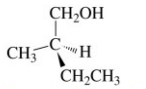
❖ **Racemic Mixture**



(*S*)-(+)-lactic acid

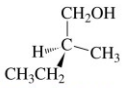


(*S*)-(–)-sodium lactate



(*R*)-2-methyl-1-butanol

$[\alpha]_D^{20\,°C} = +5.75$



(*S*)-2-methyl-1-butanol

$[\alpha]_D^{20\,°C} = -5.75$

$$\text{enantiomeric excess} = \frac{\text{observed specific rotation}}{\text{specific rotation of the pure enantiomer}} \times 100\%$$

The sample of 2-bromobutane has an observed specific rotation of +9.2°. (R)-2-bromobutane has a specific rotation of -23.1°. Calculate the enantiomeric excess $(\%e.e)$ for the synthesis.

18

18