STEREOCHEMISTRY BY

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ISOMERISM

Same MF with different chemical structure.....

Н

0—Н

H

Eg

C2H6O

Н

Н

CLASSIFICATION OF ISOMERS

STEREOISOMERS

GEOMETRICAL

CONFORMER

OPTICAL

ISOMERS

STRUCTURAL OR CONSTITUTIONAL ISOMER

- CHAIN
- POSITIONAL
- FUNCTIONAL
- METAMERS
- TAUTOMERS

WHY NEED TO STUDT STEREOCHEMISTRY ? The properties of many drugs depends on their stereochemistry:





CIS NON-ANTINEOPLASTIC DRUGS TRAN ANTINEOPLASTIC DRUGS







R-KETAMINE HALLUCINOGEN



The difference in odor between caraway seeds and mint leaves arises from two stereoisomers of carvone due to different arrangement of atoms at the carbon (*)





R-Thalidomide (sleep-inducing)

S-Thalidomide (teratogenic)



DIFFERENCE BETWEEN STRUCTURAL AND STEREOISOMER



Tetrahedral carbon, Asymmetric carbon



CONVERTION OF TETRAHEDRAL STRUCTURE INTO FISCHER PROJECTION FORMULA





CONFIGURATION

•An absolute configuration refers to the spatial arrangement of atoms of a chiral molecular entity (or groups) and its stereochemical description. It is determine by X- ray crystallography.



Methods of determining relative configuration.

Method-1 D ,L- configuration: RELATIVE CONFIGURATION Method-2 R ,S- configuration: ABSOLUTE CONFIGURATION

RELATIVE CONFIGURATION

 $\begin{array}{c} \mathsf{CHO} & \mathsf{CHO} \\ \mathsf{H}-\mathsf{C}-\mathsf{OH} & \mathsf{HO}-\mathsf{C}-\mathsf{H} \\ \mathsf{HO}-\mathsf{C}-\mathsf{H} \\ \mathsf{CH}_2\mathsf{OH} & \mathsf{CH}_2\mathsf{OH} \end{array}$

(+)-GLYCERALDEHYDE (-)-GLYCERALDEHYDE

<u>D and L Assignments</u>

CHO H OH CH₂OH

D-(+)-glyceraldehyde (D) sugar.



CHO H \mathbf{OH} HO H H OH H) HCH₂OH **D-(+)-glucose**

What is the meaning of.....

1.D-(d)-Glucose2.L-(d)-Glucose3.D-(l)-Glucose4.L-(l)-Glucose

CONFIGURATION AND THE R-S CONVENTION



Rule 1

The atoms directly attached to the stereogenic center are ranked according to atomic number. The higher the atomic number, the higher the priority



Rule 2

If a decision cannot be reached with rule 1, work outward from the stereogenic center until a decision is made. Example of ethyl and methyl below.



Rule 3

Multiple bonds are treated as if they were an equal number of single bonds.



Which group has the higher priority, isopropyl or vinyl?

$$\begin{array}{ccc} -\mathrm{CH}{=}\mathrm{CH}_2 &\equiv & -\mathrm{CH}{-}\mathrm{CH}_2\\ & & & & & & \\ \mathrm{vinyl} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & &$$

$$\begin{array}{ccc} -\text{CH}(\text{CH}_3)_2 & \equiv & -\text{CH}-\text{CH}_2\\ \text{isopropyl} & & & | & |\\ & & \text{CH}_3 & \text{H} \end{array}$$

Assign the configuration (R or S) to the following enantiomer of 3-methyl-hexane







Example: Name the following compounds.



CLASIFICATION OF STEREOISOMERS

1.OPTICAL ISOMERS

2. GEOMETRICAL ISOMERS

3. CONFORMATIONAL ISOMERS

Optical activity – When a substance rotates the plane of plane polarized light. (1815 by Biot)

Plane polarized light – Light that has been passed through a nicol prism or other polarizing medium so that all of the vibrations are in the same plane.



POLARIMETER – An instrument used to measure optical activity.





DEXTROROTATORY – when the plane of polarized light is rotated in a clockwise direction when viewed through a polarimeter.

(+) or (*d*) do not confuse with D **LEVOROTATORY** – when the plane of polarized light is rotated in a counter-clockwise direction when viewed through a polarimeter.

(-) or (*I*) do not confuse with L

The angle of rotation of plane polarized light by an optically active substance is proportional to the number of atoms in the path of the light.

Stereoselective and stereospecific reactions.

 $CH_3CH=CHCH_3 + Br_2 \rightarrow CH_3CHCHCH_3$ Br Br

2-butene

2 geometric isomers *cis-* and *trans-* 3 stereoisomers (*S*,*S*)-, (*R*,*R*)-, and (*R*,*S*)*meso*-

2,3-dibromobutane



MESO-2,3-DIBROMOBUTANE

A reaction in which stereochemically different molecules react differently is called a stereospecific reaction. In this case the *cis-* and *trans*stereoisomers give different products.



PRODUCT IS RACEMIC MIXTURE

HOMOTOPIC ATOMS



ENANTIOTOPIC ATOM



DIASTEREOTOPIC ATOM



PRODUCTS ARE DIASTEREOMERS OF EACH OTHER

THANK YOU