

November 11-15 Notes

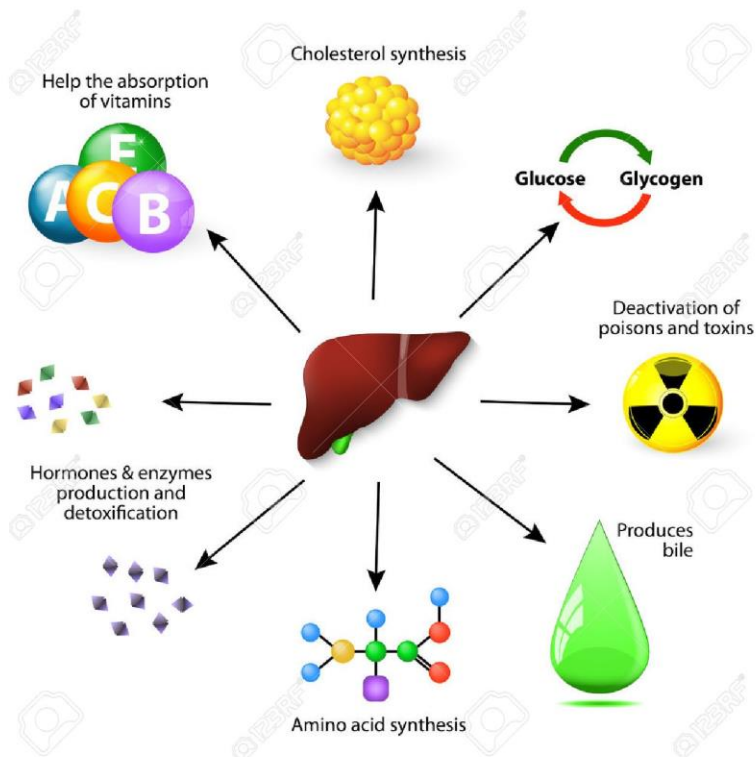
Video 27: Conformation of alkanes

Video 28: Functional groups

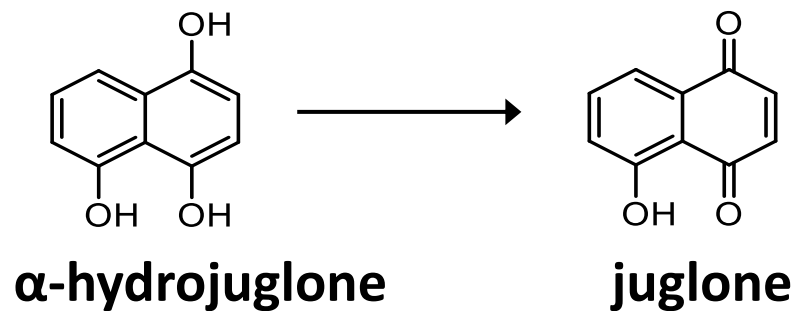
Video 29: Stereochemistry and isomers

Why do we care about organic chemistry?

Understanding chemistry of life around us!



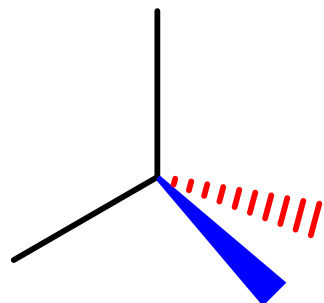
Metabolism



Plant defense

Conformation

Conformation – The different three-dimensional structures that can be adopted – rotation of atoms about **single bonds**



Solid Line

Wedged Bond: bond is pointing forward

Dashed Bond: bond is pointing away

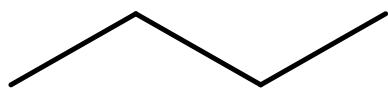


sp³ hybrid orbitals
tetrahedral

Tetrahedral – sp³ geometry

Sawhorse projection

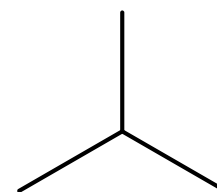
Conformation – The different three-dimensional structures that can be adopted – rotation of atoms about **single bonds within the same molecule**



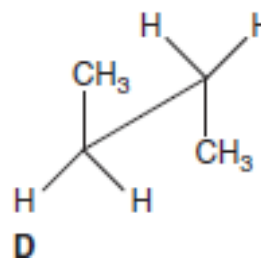
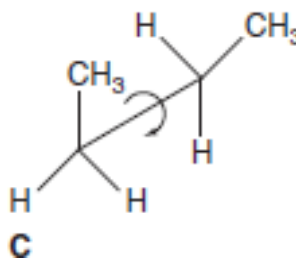
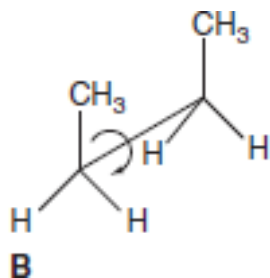
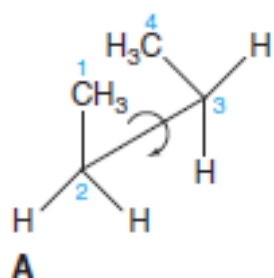
Butane, C_4H_{10}



Butane, C_4H_{10}



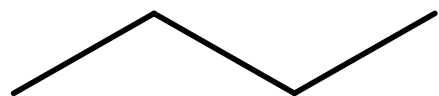
2-methylpropane, C_4H_{10}
NOT SAME MOLECULE
(structural isomer)



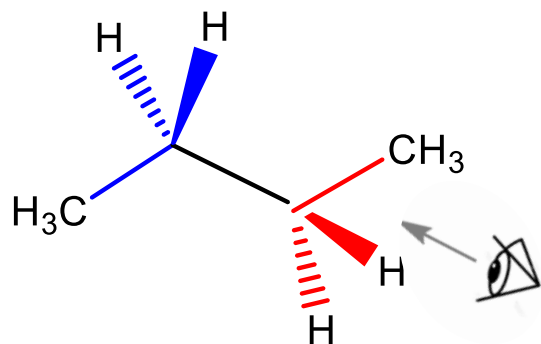
Sawhorse projection of butane --- all the SAME molecule!

Newman Projection

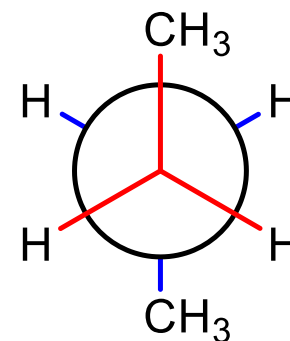
Conformation – The different three-dimensional structures that can be adopted – rotation of atoms about **single bonds**



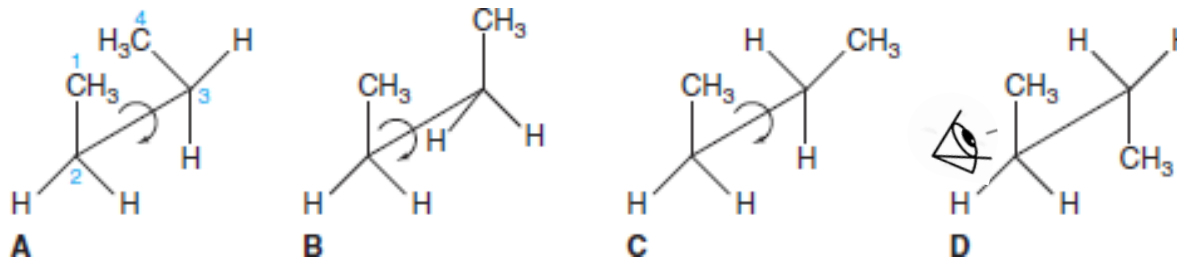
Butane - skeletal



Butane –
showing the conformation

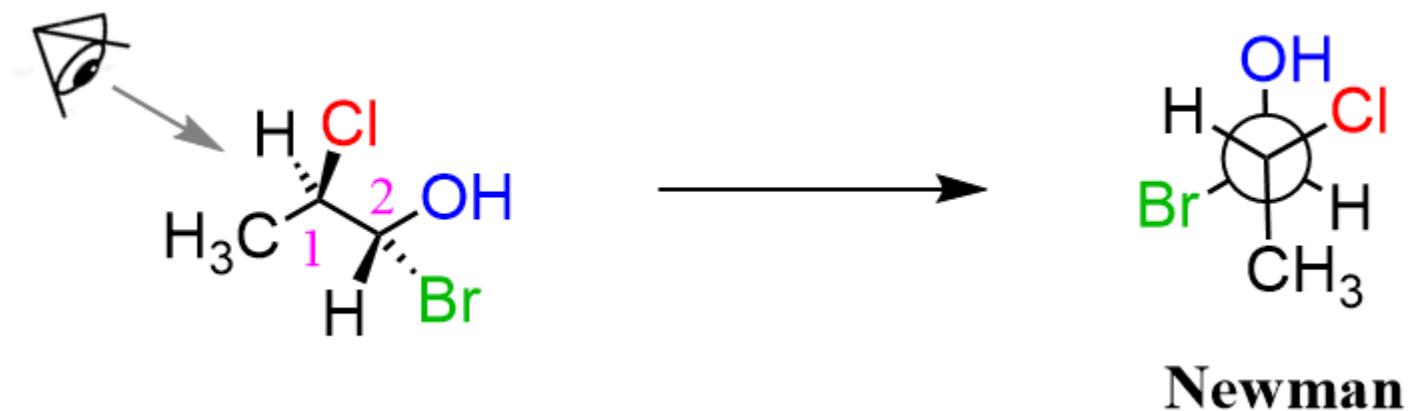


Newman projection
of butane

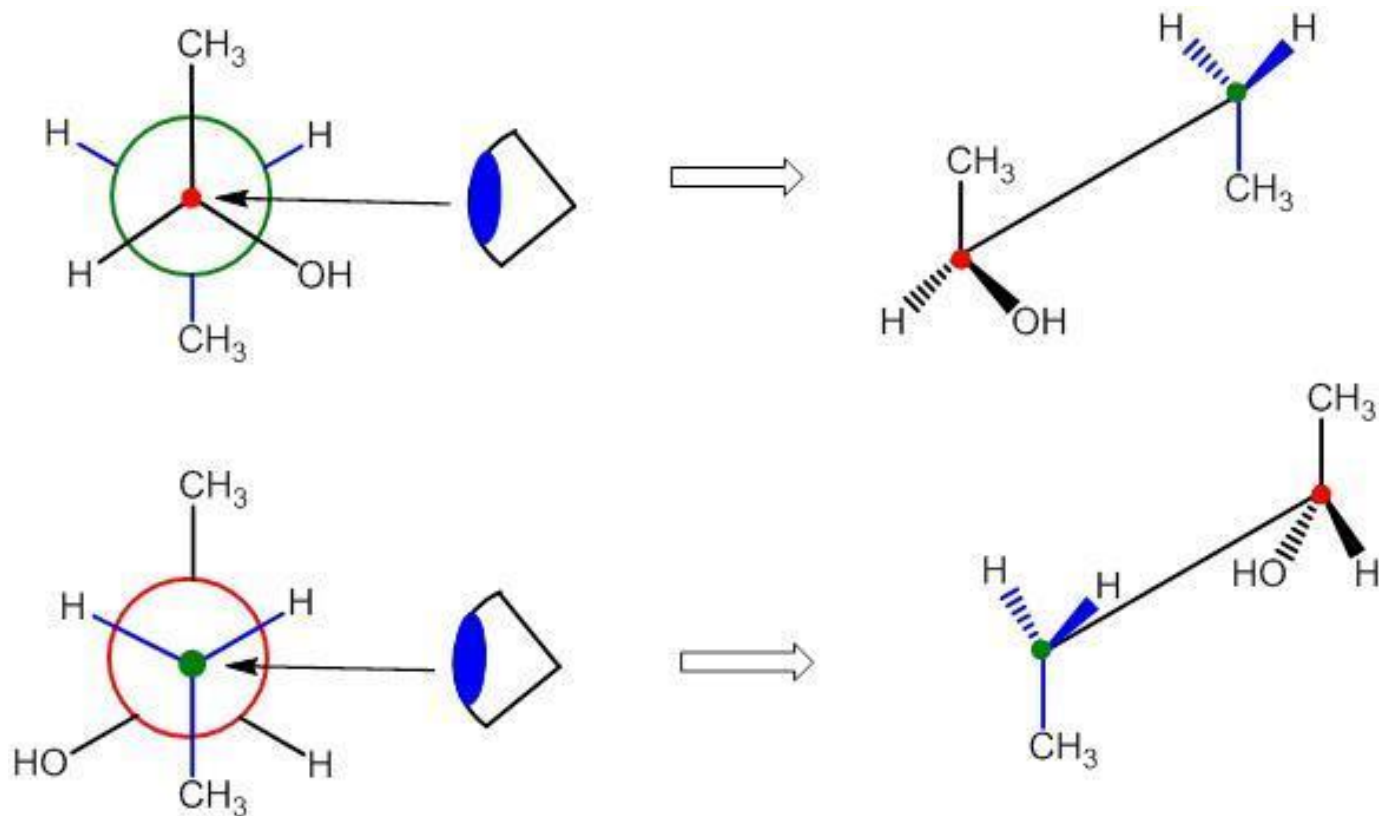


Sawhorse projection of butane

Another Newman Project example

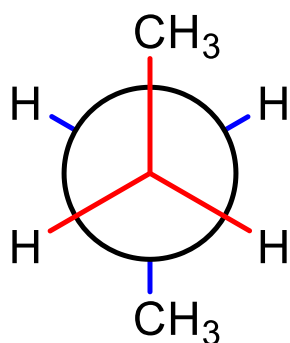


Newman Projection and sawhorse

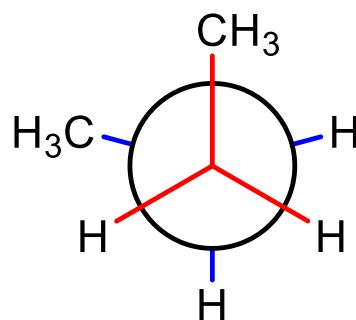


Conformation Changes and Potential Energy

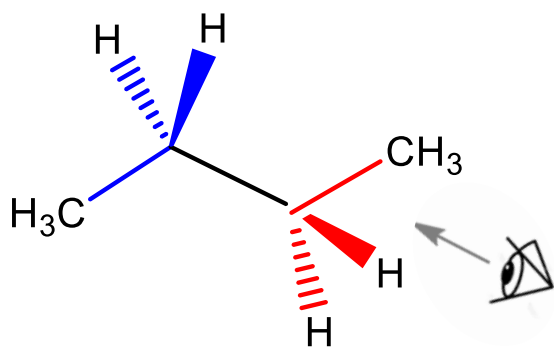
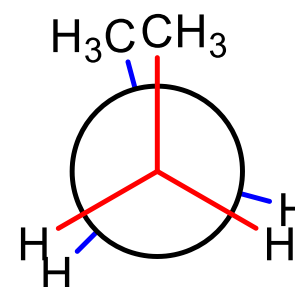
Rotation along the C-C bond:



staggered



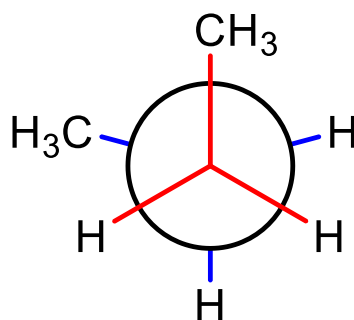
eclipsed



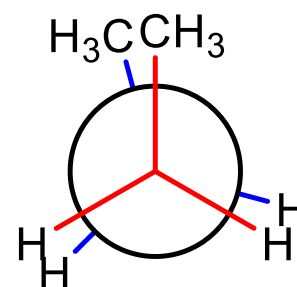
Conformation Changes and Potential Energy

Eclipsed is not stable, it is only a transition state

staggered

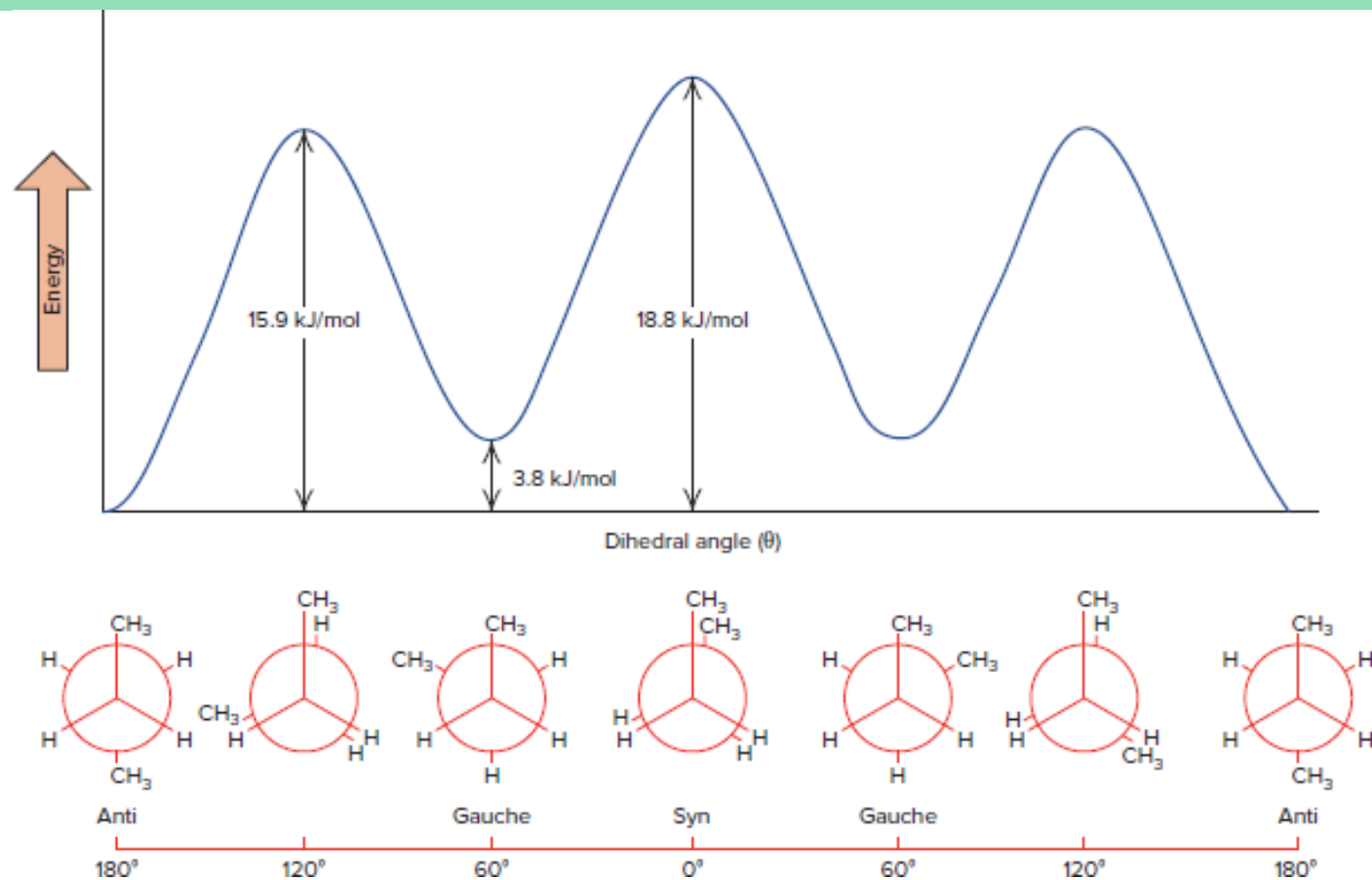


eclipsed



Structures that are “eclipsed” suffer from steric strain (or eclipsed strain)

Chain alkane can rotate around the bonds to achieve the most stable conformation



The conformations have different energy – lowest energy for the conformation where the **two GIANT CH₃ groups are furthest apart from each other**

Extra video to help you visualize

Newman projection:

<https://www.youtube.com/watch?v=ETqgo9rAO80>

And more on youtube 😊








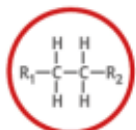
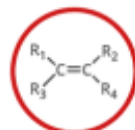
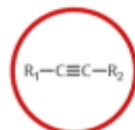
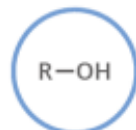
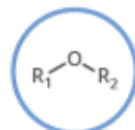
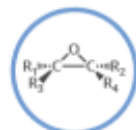

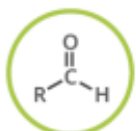
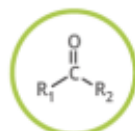
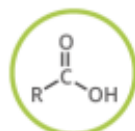
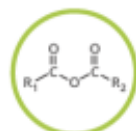
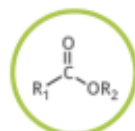
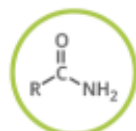
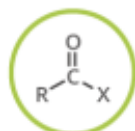
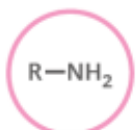

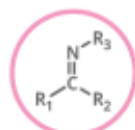

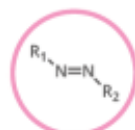

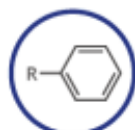
Nov 11-15

Video 28: Functional groups

Functional Groups!!!!!!!!!!

FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.

 HYDROCARBONS	 SIMPLE OXYGEN HETEROATOMICS	 HALOGEN HETEROATOMICS	 CARBONYL COMPOUNDS	 NITROGEN-BASED	 SULFUR-BASED	 AROMATIC
 ALKANE Naming: -ane e.g. ethane	 ALKENE Naming: -ene e.g. ethene	 ALKYNE Naming: -yne e.g. ethyne	 ALCOHOL Naming: -ol e.g. ethanol	 ETHER Naming: -oxy-ane e.g. methoxyethane	 EPOXIDE Naming: -ene oxide e.g. ethene oxide	 HALOALKANE Naming: halo- e.g. chloroethane
 ALDEHYDE Naming: -al e.g. ethanal	 KETONE Naming: -one e.g. propanone	 CARBOXYLIC ACID Naming: -oic acid e.g. ethanoic acid	 ACID ANHYDRIDE Naming: -oic anhydride e.g. ethanoic anhydride	 ESTER Naming: -yl -oate e.g. ethyl ethanoate	 AMIDE Naming: -amide e.g. ethanamide	 ACYL HALIDE Naming: -oyl halide e.g. ethanoyl chloride
 AMINE Naming: -amine e.g. ethanamine	 NITRILE Naming: -nitrile e.g. ethanenitrile	 IMINE Naming: -imine e.g. ethanimine	 ISOCYANATE Naming: -yl isocyanate e.g. ethyl isocyanate	 AZO COMPOUND Naming: azo- e.g. azoethane	 THIOL Naming: -thiol e.g. methanethiol	 ARENE Naming: -yl benzene e.g. ethyl benzene



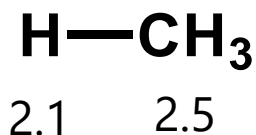
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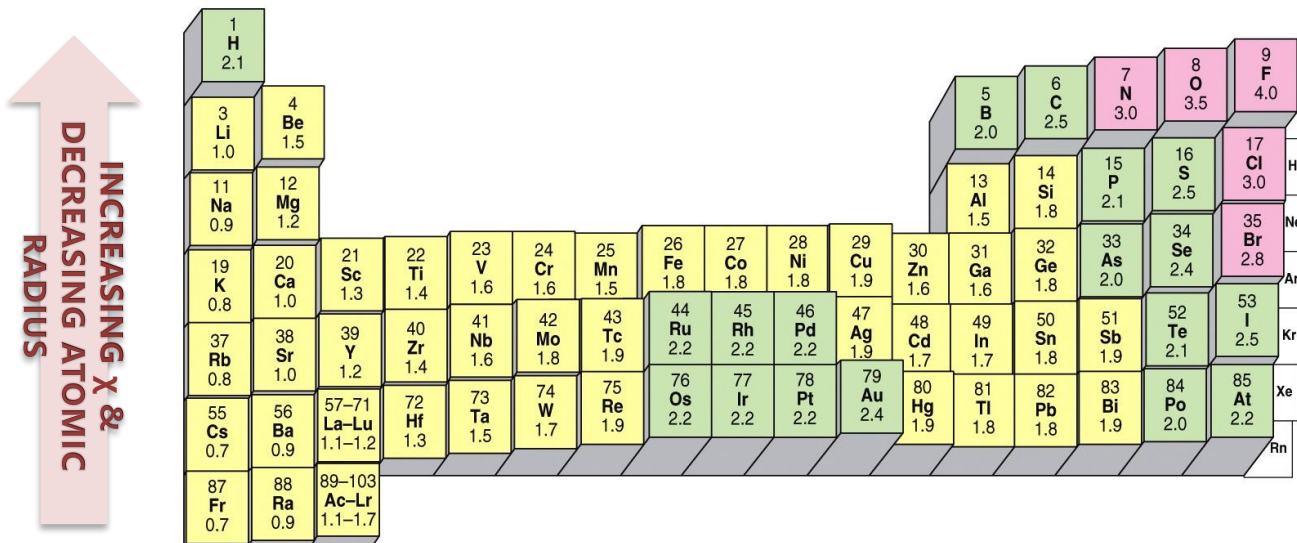
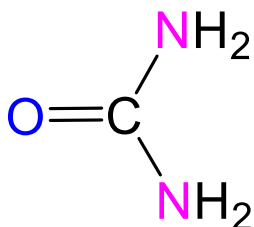
Functional groups = i.e. give the molecule "function"

Hydrocarbons and electronegativity

Electronegativity – ability of an element to attract bonding electrons



$\Delta\chi$
0.4



Heteroatoms

- Oxygen
- Nitrogen
- Phosphorus
- Sulfur
- Halides

Also result in new intermolecular forces
(i.e. H-bonds!)

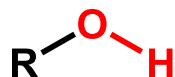


We will look at 10 classes of molecules containing different functional groups

SATURATED

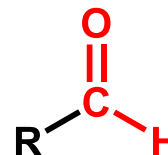


Saturated
Halide

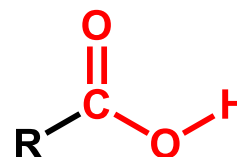


Saturated
Alcohol

UNSATURATED



Unsaturated
Aldehyde

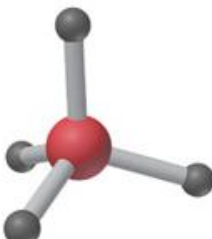
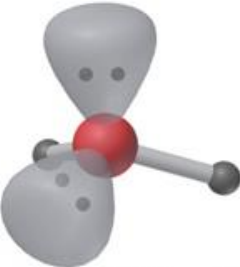



Unsaturated
Carboxylic Acid

R is a general symbol that represents an **ALKYL** group
(i.e. any hydrocarbon)

We do this so we focus on the chemistry happening at the functional group (simplify)

Saturated Functional Groups

Group Functional group	HALO (Halide) $R-X$	HYDROXYL (Alcohol) $R-O-H$	ALKOXY (Ether) $R-O-R$	AMINO (Amine) $R-N(R)(R)$
				
	Tetrahedral	Bent (V shaped)		Trigonal pyramidal

Halides:

F

Cl

I

Br...

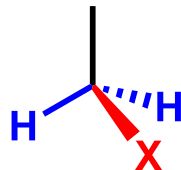
We are focusing on the *functional* group, but it is useful to know the different structural groups involved

Functional Groups: 1. Halides

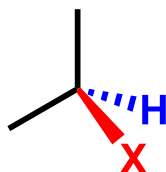
Saturated Functional Groups

HALO
 $\text{R}-\text{X}$

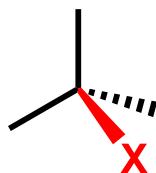
X = any halogen (i.e. F, Br, I, Cl)



1° halide : Primary Halide
(1° carbon)



2° halide: Secondary halide
(2° carbon)



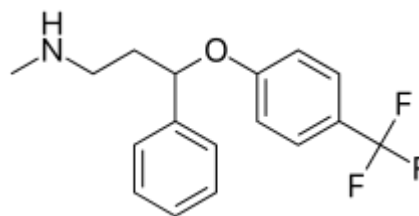
3° halide: Tertiary halide
(3° carbon)

Notice how they are classified as primary, secondary etc based on the carbon they are attached to!

Functional Groups: 1. Halides

Saturated Functional Groups

Naturally occurring organofluorine compounds are rare
-but 20% of all pharmaceuticals contain fluorine, including Prozac.

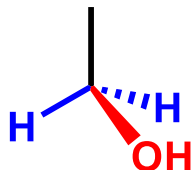
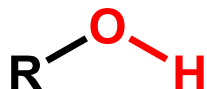


Functional Groups: 2. Alcohols

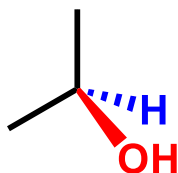
I'm sure I don't need to give an example of an alcohol.....

Saturated Functional Groups

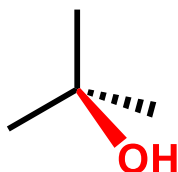
HYDROXYL
(Alcohol)



1° alcohol : Primary Alcohol
(1° carbon)



2° alcohol: Secondary Alcohol
(2° carbon)



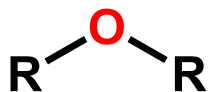
3° alcohol: Tertiary alcohol
(3° carbon)

Notice again that
they are classified
as primary,
secondary etc
based on the carbon
they are attached to!

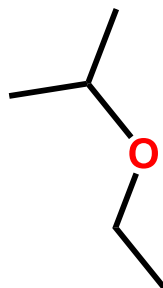
Functional Groups: 3. Ether

Saturated Functional Groups

ALKOXY
(Ether)



Symmetrical Ether

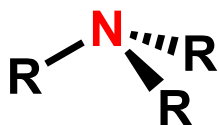


Asymmetrical Ether

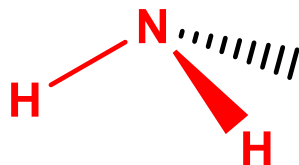
Functional Groups: 4. Amines

Saturated Functional Groups

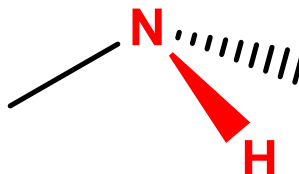
AMINO



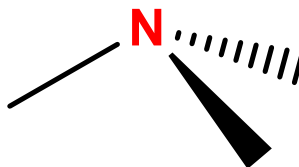
NOTE! NOT based on the carbon at all! Focus on the nitrogen! Based on how many carbons the nitrogen is attached TO. So 1 carbon bonded to the nitrogen = primary; 3 carbons on the nitrogen = tertiary



1° amine : Primary Amine
(1° nitrogen)



2° amine: Secondary Amine
(2° nitrogen)

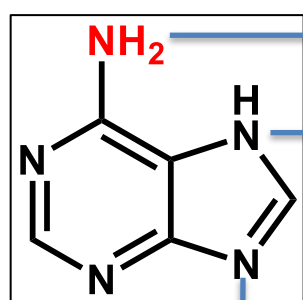


3° amine: Tertiary amine
(3° nitrogen)

Functional Groups: 4. Amines

Saturated Functional Groups

Nitrogens with a double bond are NOT amino groups!



Primary amine

Not an amine

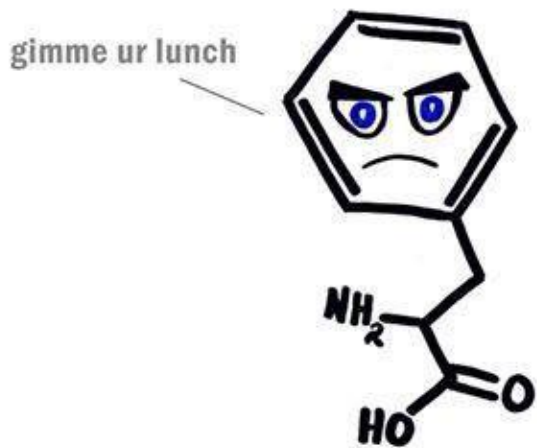
This one is tricky (due to resonance)

Not an amine

Functional Groups: 4. Amines

Amines are super important!

WHAT DO YOU CALL AN
ACID WITH AN ATTITUDE?



THE CHEMICAL STRUCTURE OF DNA

THE SUGAR PHOSPHATE 'BACKBONE'

DNA is a polymer made up of units called nucleotides. The nucleotides are made of three different components: a sugar group, a phosphate group, and a base. There are four different bases: adenine, thymine, guanine and cytosine.

WHAT HOLDS DNA STRANDS TOGETHER?

DNA strands are held together by hydrogen bonds between bases on adjacent strands. Adenine (A) always pairs with thymine (T), while guanine (G) always pairs with cytosine (C). Adenine pairs with uracil (U) in RNA.

FROM DNA TO PROTEINS

The bases on a single strand of DNA act as a code. The letters form three letter codons, which code for amino acids - the building blocks of proteins.

DNA → TRANSCRIPTION → **RNA** → TRANSLATION → **PROTEIN**

An enzyme, RNA polymerase, transcribes DNA into mRNA (messenger ribonucleic acid). It splits apart the two strands that form the double helix, then reads a strand and copies the sequence of nucleotides. The only difference between the DNA and the original DNA is that in the place of thymine (T), another base with a similar structure is used: uracil (U).

DNA SEQUENCE	mRNA SEQUENCE	AMINO ACID
TTCCTGAA	UUGACG	Phenylalanine
CGGCTTAA	ACCAU	Leucine
CGGCTTAA	ACCAU	Leucine

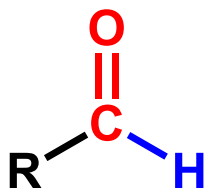
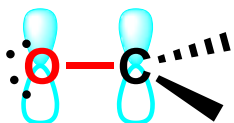
In multicellular organisms, the mRNA carries genetic code out of the cell nucleus, to the cytoplasm. Here, protein synthesis takes place. Translation is the process of turning the mRNA's code into proteins. Molecules called ribosomes carry out this process, building up proteins from the amino acids coded for.

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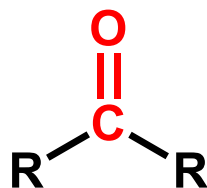
Functional Groups

Unsaturated Functional Groups

CARBONYL



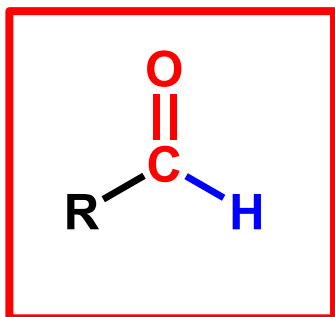
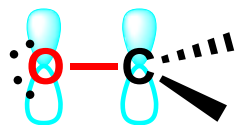
aldehyde



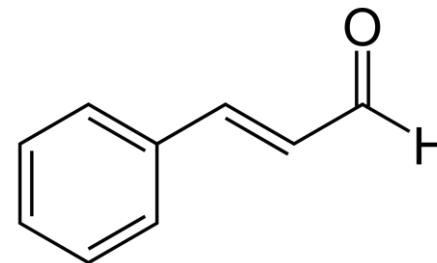
ketone

Functional Groups: 5. Aldehyde

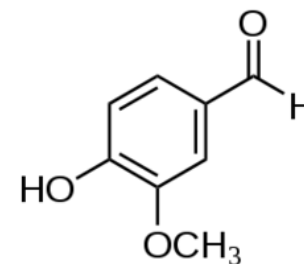
Unsaturated Functional Groups



Aldehyde: RCHO



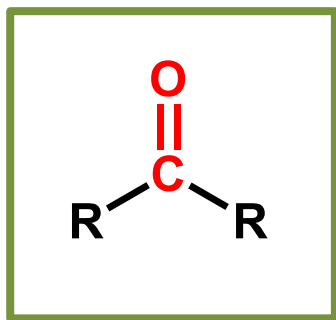
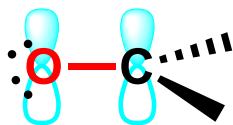
Cinnamaldehyde



Vanillin

Functional Groups: 6. Ketone

Unsaturated Functional Groups



Ketone: RCOR

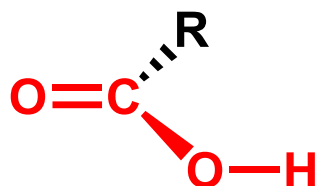
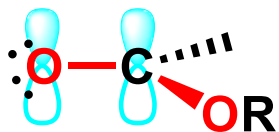
Ketosis

TYPES OF KETONE BODIES		
There are three types of ketones produced when the body goes into ketosis:		
ACETOACETATE Created first from the breakdown of fatty acids. It's either converted into BHB or spontaneously turned into acetone.	BETA-HYDROXYBUTYRIC ACID (BHB) Formed from acetoacetate. BHB is not technically a ketone because of its structure, but we consider it as one within the keto diet.	ACETONE Created spontaneously as a side product of acetoacetate. Breaks down quickly and is removed from the body through the waste or the breath.
PERFECT KETO		

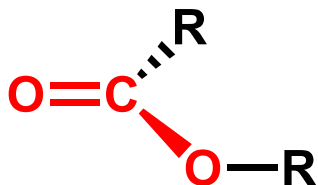
Functional Groups

Unsaturated Functional Groups

CARBOXYL



Carboxylic acid

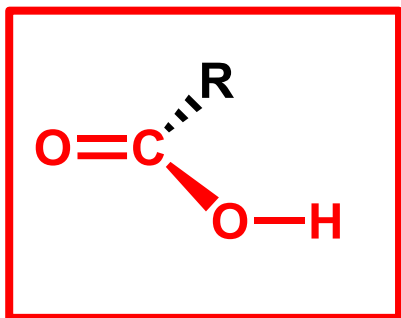
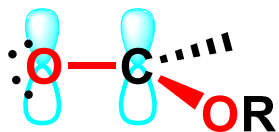


ester

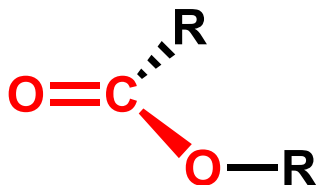
Functional Groups: 7. Carboxylic Acid

Unsaturated Functional Groups

CARBOXYL



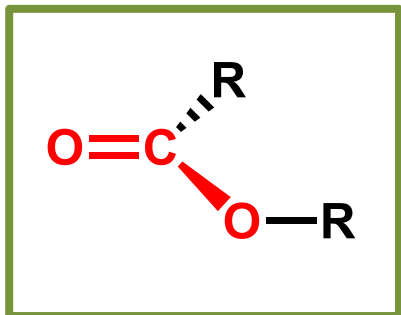
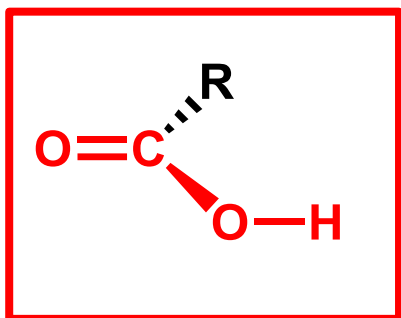
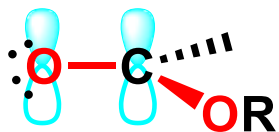
Carboxylic Acid: RCOOH



Functional Groups: 8. Ester

Unsaturated Functional Groups

CARBOXYL



Carboxylic Acid: RCO_2H

Ester: RC(O)OR

Acetic acid
(ethanoic acid)

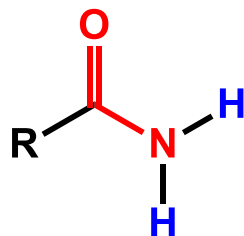
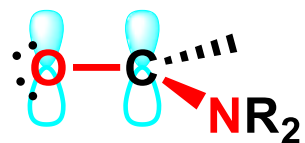


Examples:
-fruity smells
-see page 916

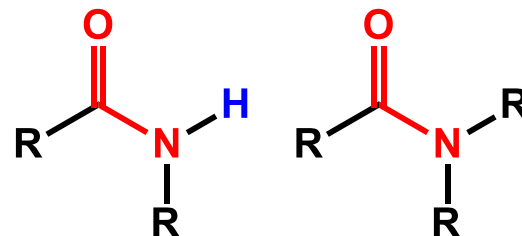
Functional Groups: 9. Amide

Unsaturated Functional Groups

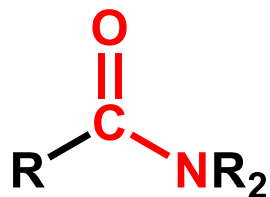
AMIDO



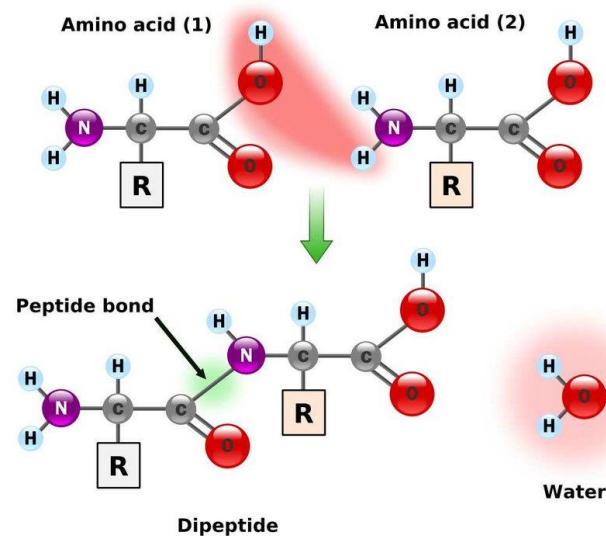
unsubstituted
amides



substituted amides



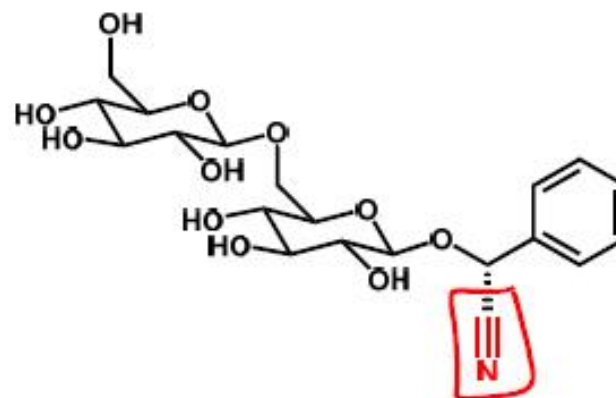
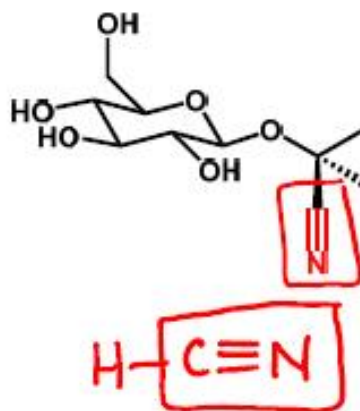
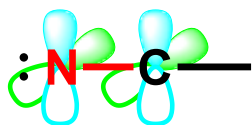
Amides: RCONR_2



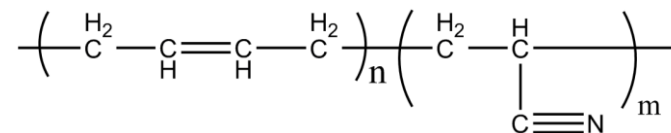
Functional Groups: 10. Nitriles

Unsaturated Functional Groups

CYANO

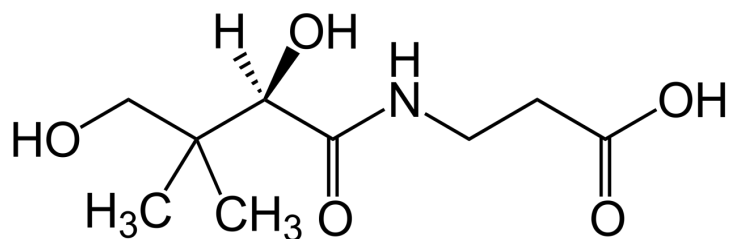


Nitrile
RCN

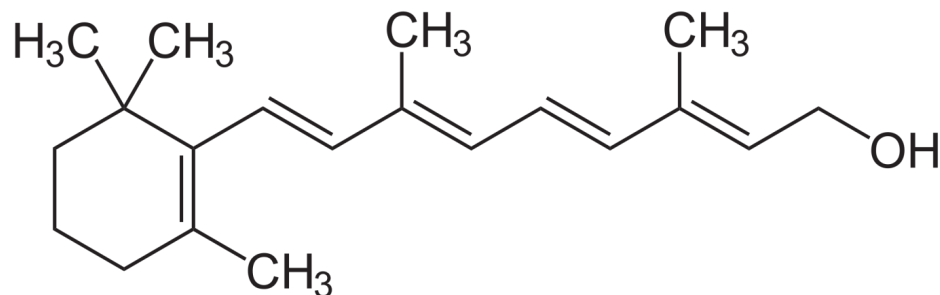


Functional Groups in Biological Compounds: PRACTICE

Circle and name the functional groups



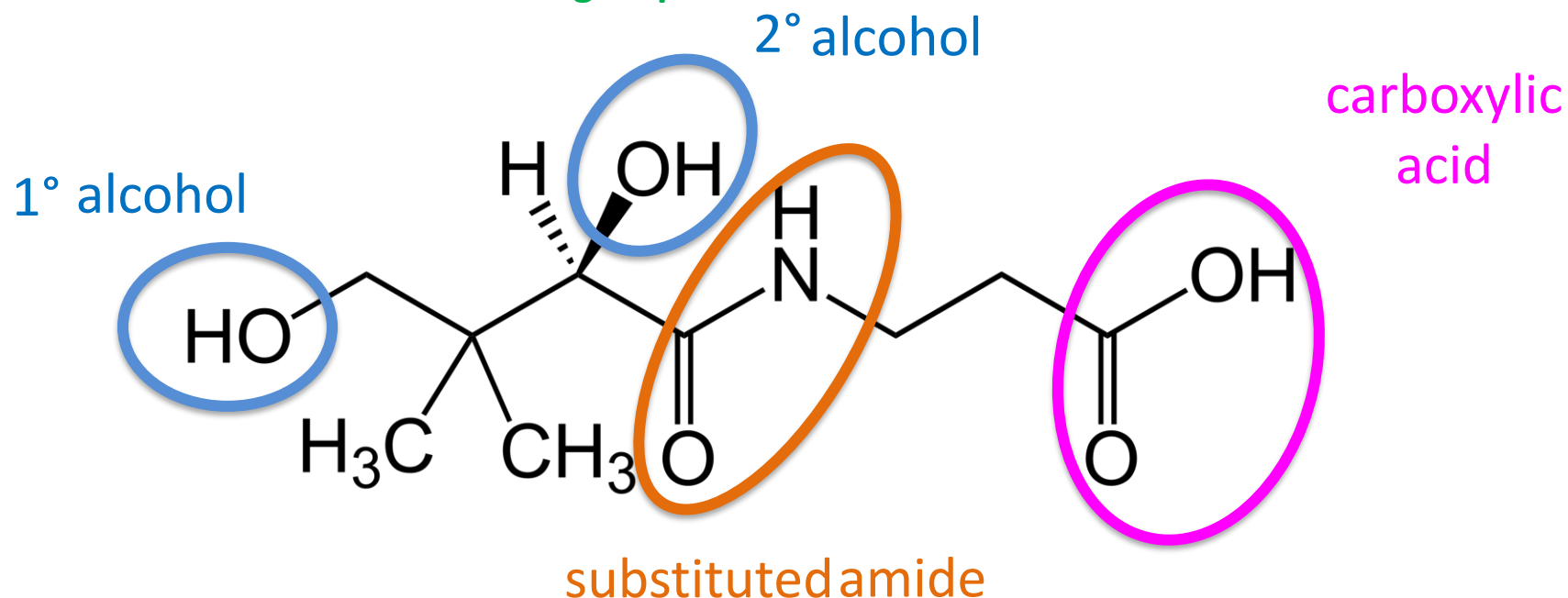
Vitamin B5
(pantothenic acid)



Vitamin A1
(retinol)

Functional Groups in Biological Compounds: PRACTICE

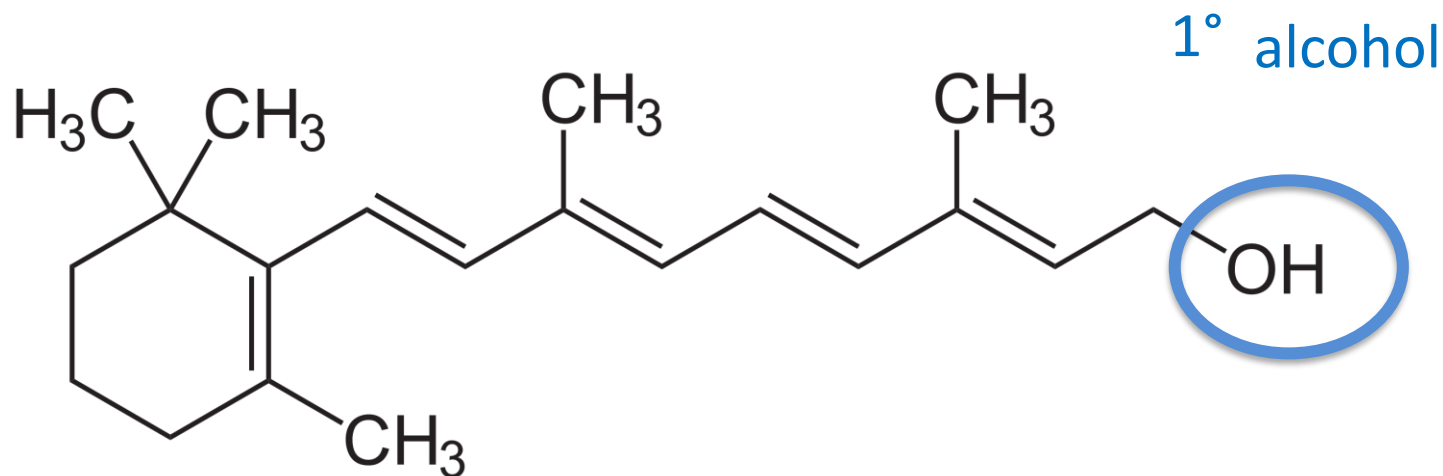
Circle and name the functional groups



Vitamin B5
(pantothenic acid)

Functional Groups in Biological Compounds: PRACTICE

Circle and name the functional groups

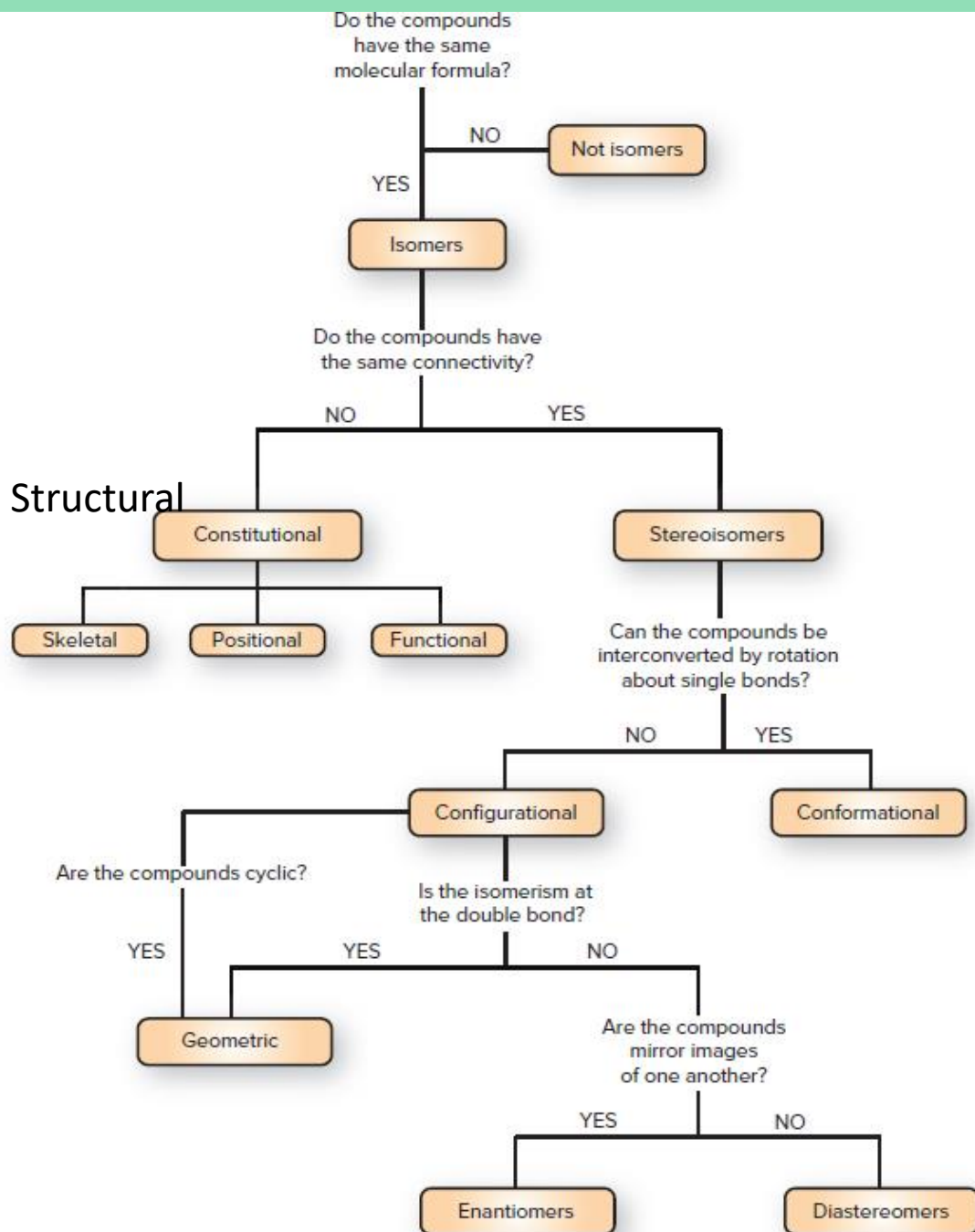


Vitamin A1
(retinol)

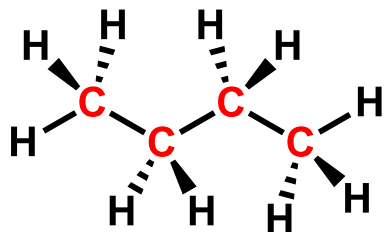
Video 29: Stereochemistry and isomers

Isomers!

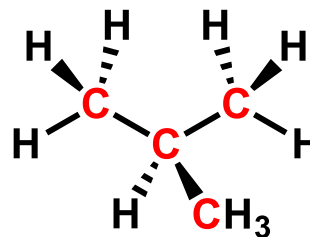
also called Structural



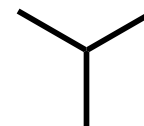
Different kinds of structural isomers



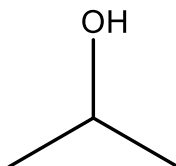
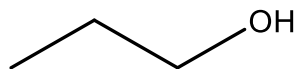
BUTANE



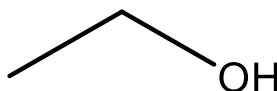
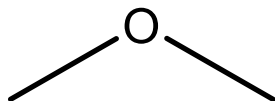
ISOBUTANE



Same chemical formula different arrangement of carbon atoms – SKELETAL ISOMERS

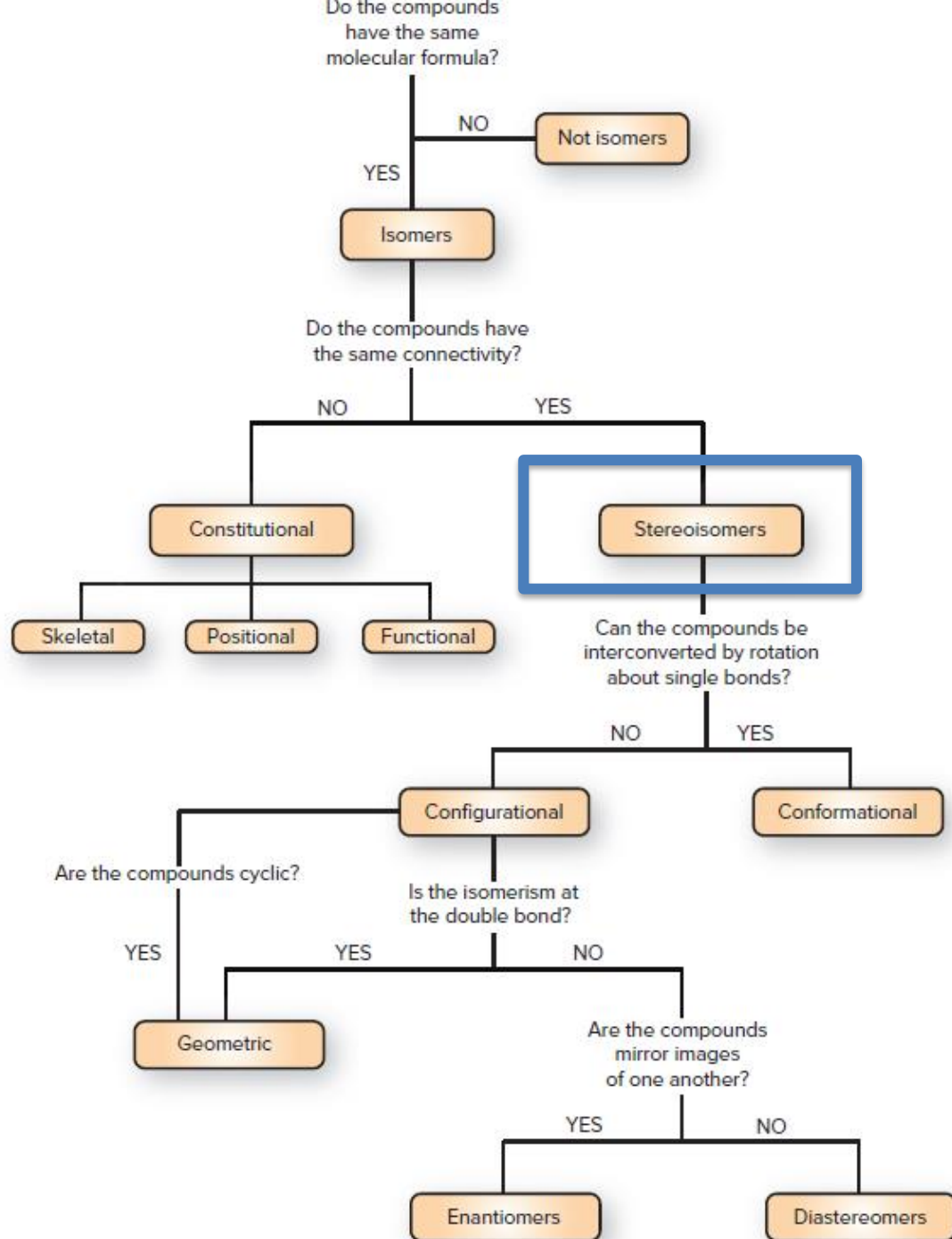


Same chemical formula different position of functional group – POSITIONAL ISOMERS



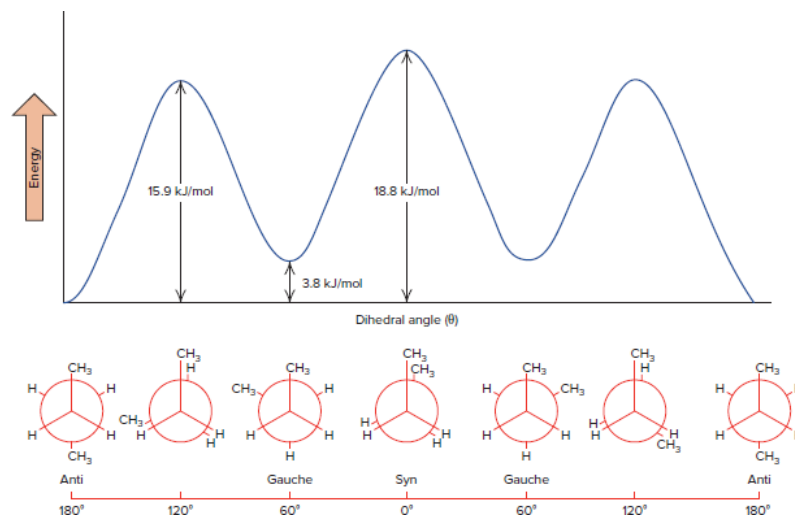
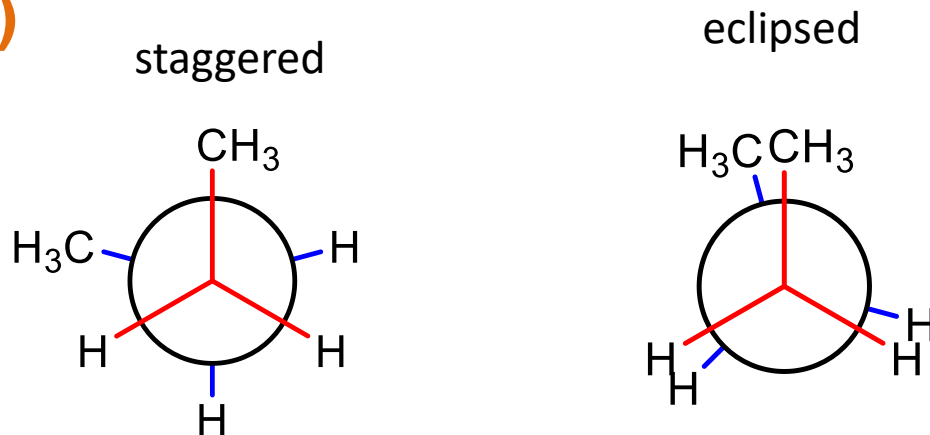
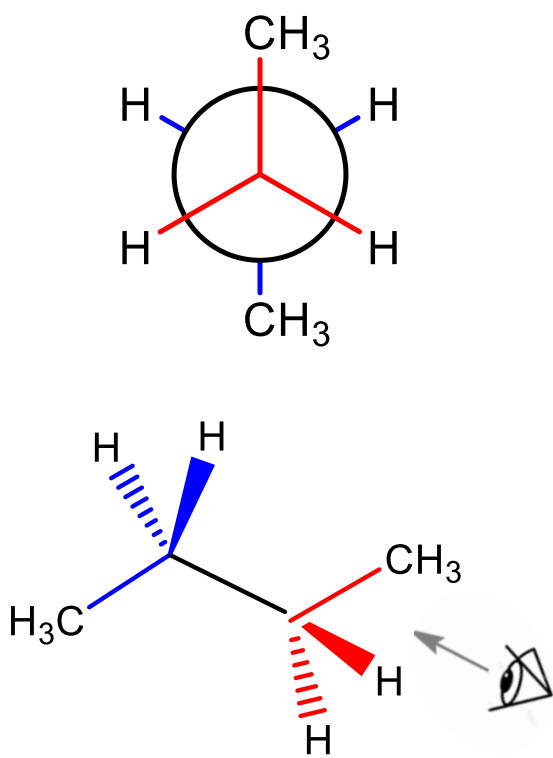
Same chemical formula different functional groups – FUNCTIONAL ISOMERS

Isomers!



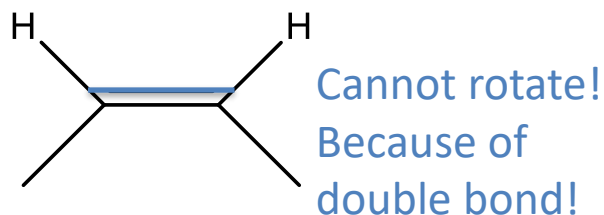
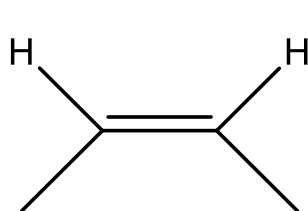
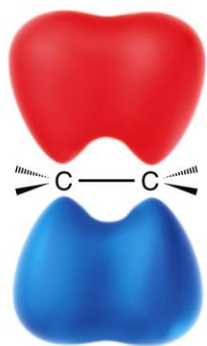
Conformation Changes and Potential Energy

Reminder these are all conformational isomers of each other (really just the same molecule in different conformation)



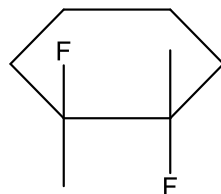
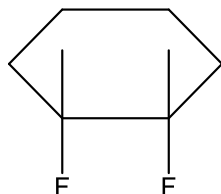
Conformation Changes in Alkanes

Conformation – The different three-dimensional structures that can be adopted – rotation of atoms about **single bonds**



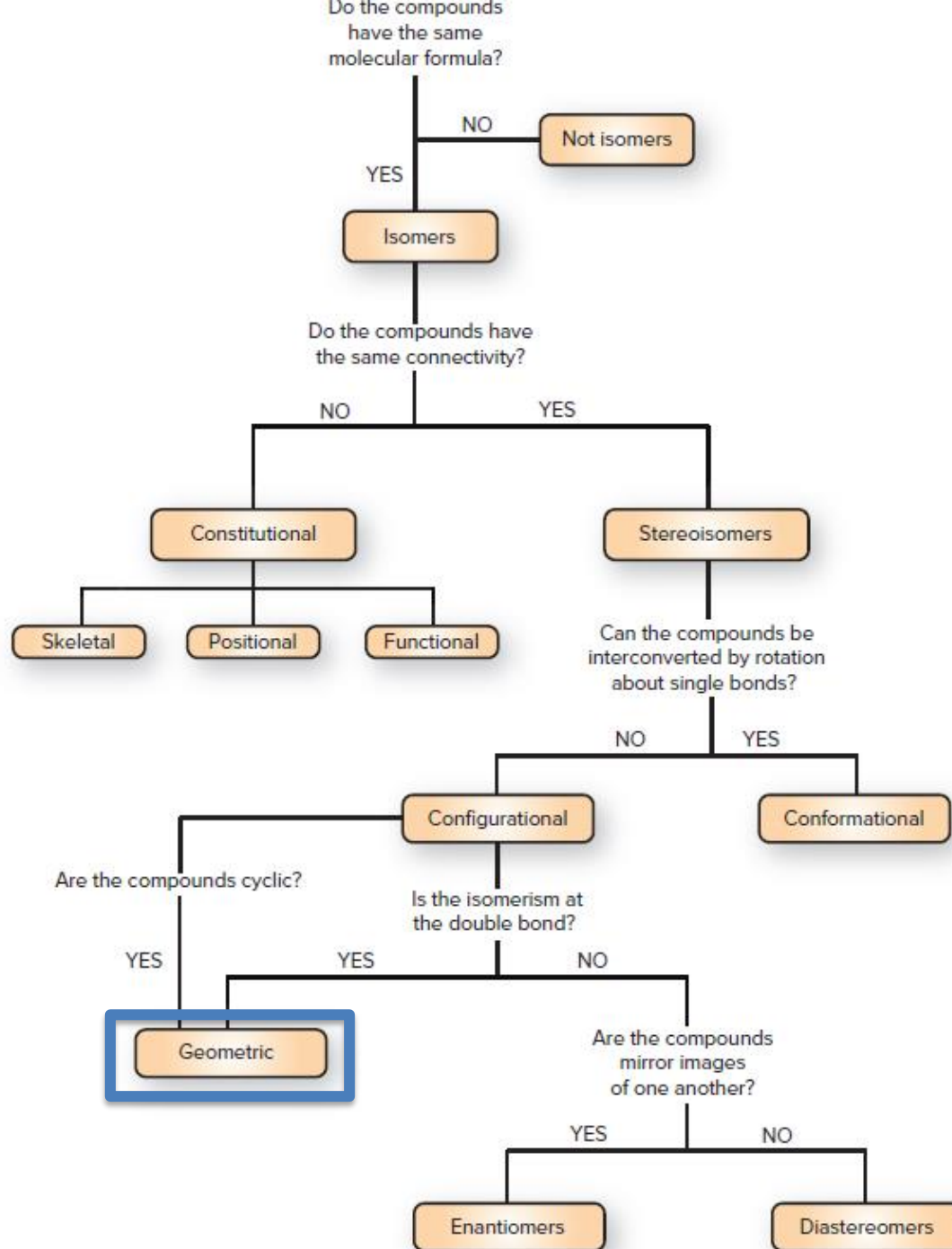
π -bond – above and below C-C σ -bond axis (nodal plane)

- unpaired electrons from p_z orbitals overlap side-to-side
- two electrons can move over new π -bonding molecular orbital
- **no C-C bond rotation, would have to break π -bond**

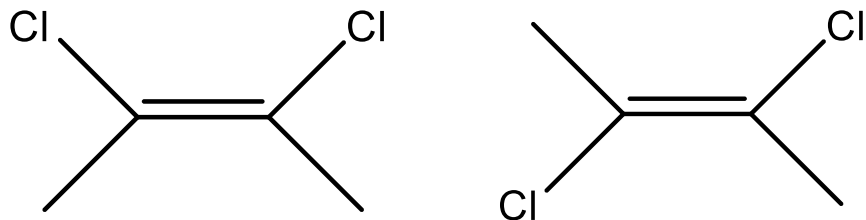


Also can't rotate bonds in a cyclic molecule without breaking bonds

Isomers!



Naming geometric Isomers



Geometrical isomers of organic molecules are distinguished by the prefixes cis- (same side) and trans- (across)

Cis = majority of **CARBON** chain on the same side

Trans = majority of the carbon chain on opposite sides

The more correct and common nomenclature is “E/Z”.

E = entgegen (opposite)

Z = zusammen (together)

E/Z based on “priority” not based on carbon chain length!

-priority = “heaviest” i.e. highest atomic number

Naming geometric Isomers

Cis = majority of chain on the same side

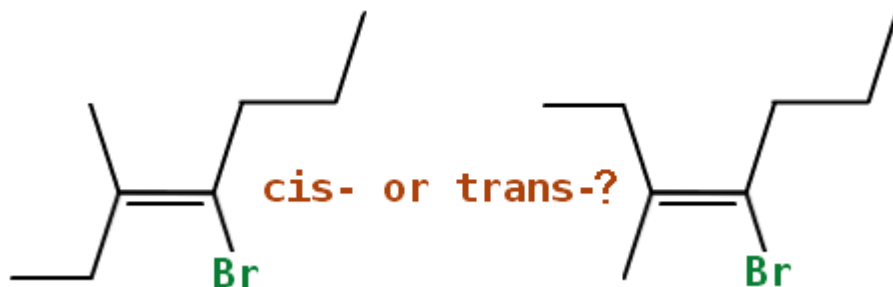
Trans = majority of the carbon chain on opposite sides

Not always the same!!!

E = entgegen (opposite)

Z = zusammen (together)

E/Z based on “priority” not based on chain length!



Naming geometric Isomers

Cis = majority of chain on the same side

Trans = majority of the carbon chain on opposite sides

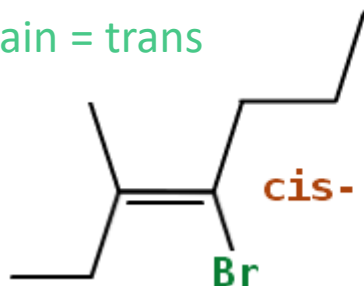
Not always the same!!!

E = entgegen (opposite)

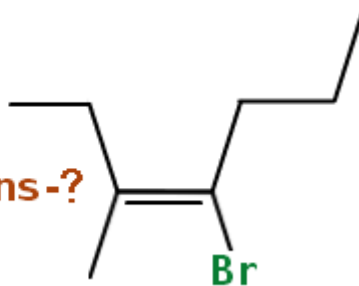
Z = zusammen (together)

E/Z based on “priority” not based on chain length!

Longest chain = trans



cis- or trans-?



Longest chain = cis

Naming geometric Isomers

Cis = majority of chain on the same side

Trans = majority of the carbon chain on opposite sides

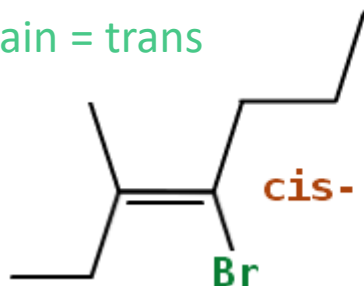
Not always the same!!!

E = entgegen (opposite)

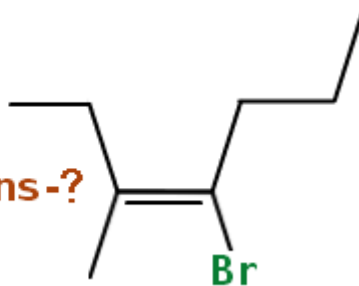
Z = zusammen (together)

E/Z based on “priority” not based on chain length!

Longest chain = trans



cis- or trans-?



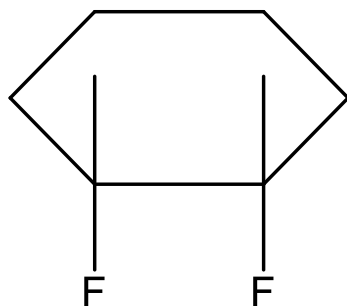
Longest chain = cis

Highest priority is opposite (E)

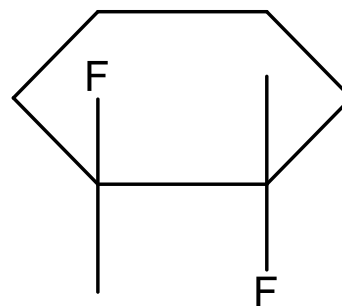
Highest priority is on the same side (Z)

Geometric Isomers (more examples)

Same chemical formula same bonding different orientation of atoms –
STEREISOMERS



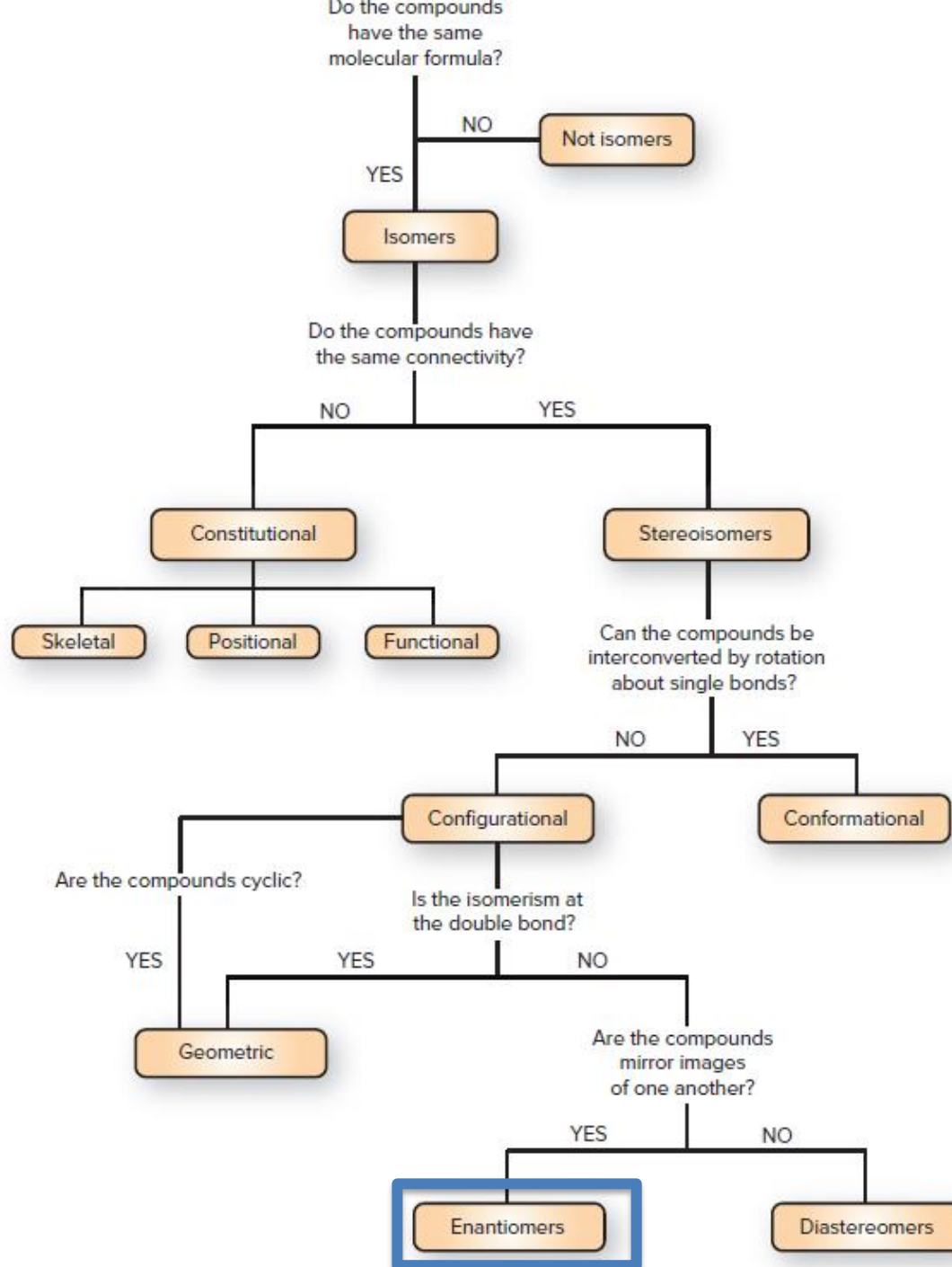
cis



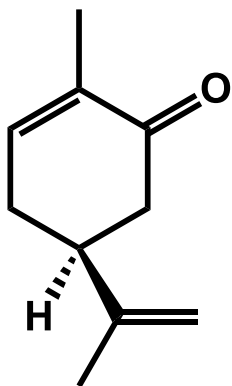
trans

Same chemical formula same bonding different rotation around a bond (not
mirror images) – GEOMETRIC ISOMERS

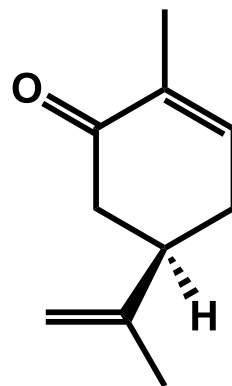
Isomers!



STEREISOMERS 2. Enantiomers



caraway

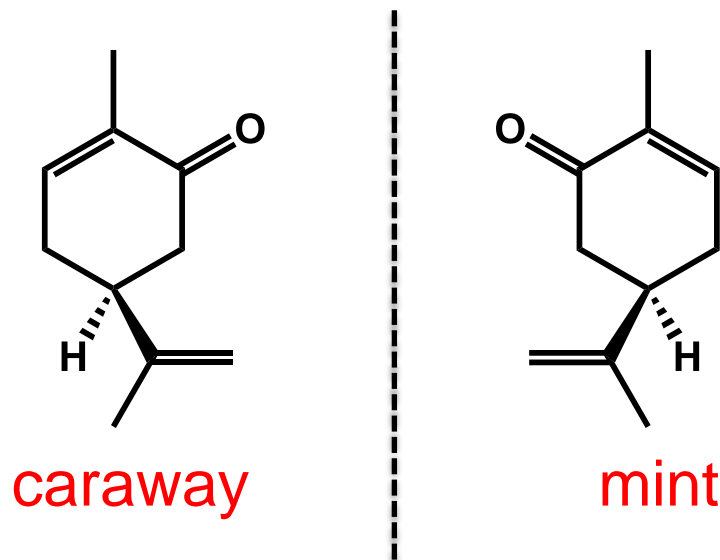


mint



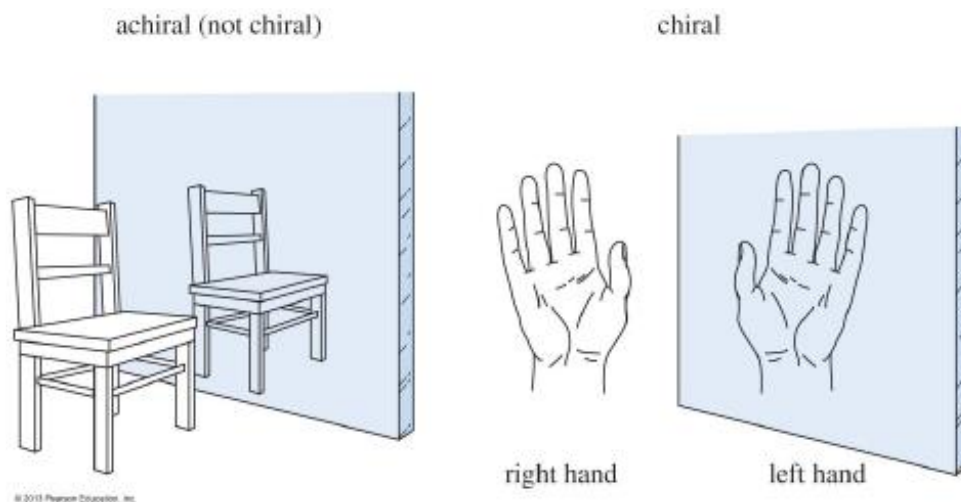
Same chemical formula same bonding nonsuperimposable mirror images –
Enantiomers

ENANTIOMERS AND CHIRALITY



CHIRAL OBJECT – one with a non-superimposable mirror image
Enantiomers are a pair of chiral objects

CHIRALITY



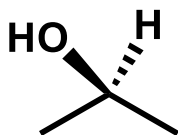
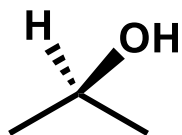
CHIRAL OBJECT – one with a non-superimposable mirror image

WATCH this video: <https://www.khanacademy.org/science/organic-chemistry/stereochemistry-topic/chirality-r-s-system/v/chiral-achiral-jay>

WHAT MAKES A MOLECULE CHIRAL?

CHIRAL MOLECULE

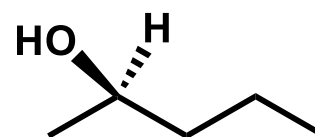
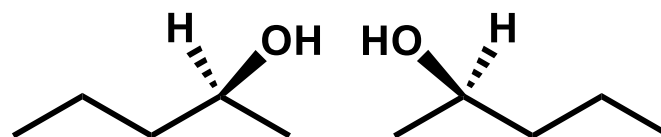
1. No plane of symmetry (can't cut it in half, or thirds etc, and get the same on one side as the other side!)
2. Must have a chiral center- 4 different groups (sp^3 hybridized)



2-propanol

ACHIRAL

SUPERIMPOSABLE
MIRROR IMAGES

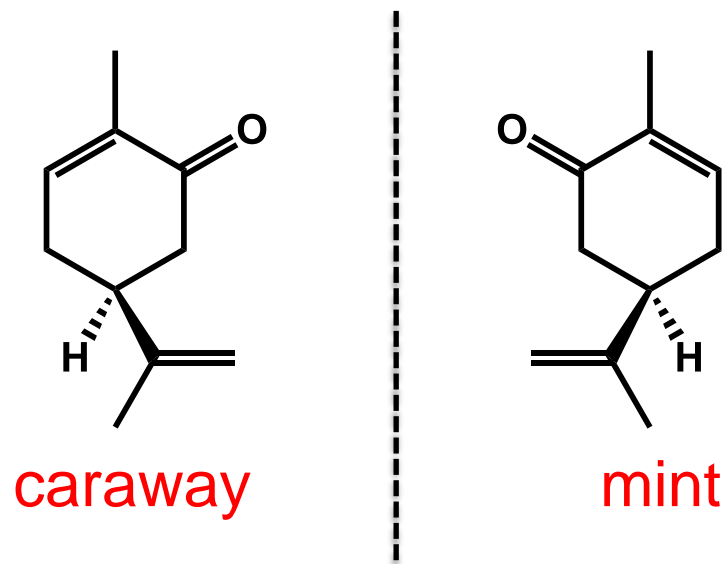


2-pentanol

CHIRAL

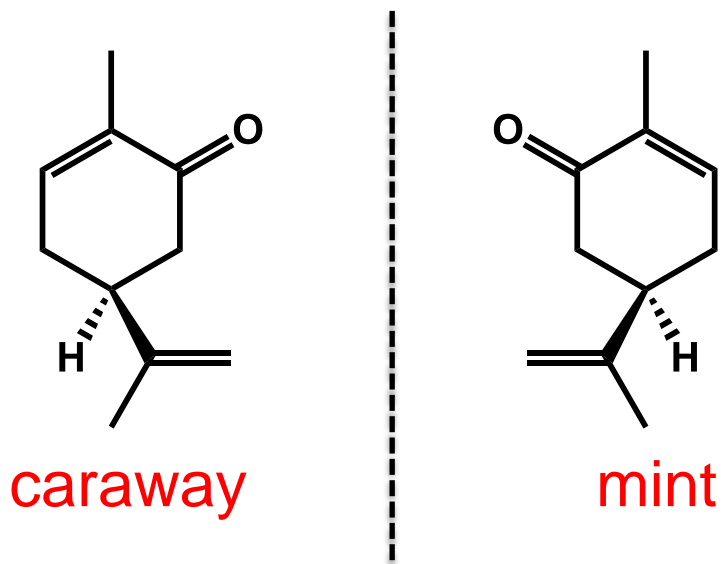
NON-SUPERIMPOSABLE
MIRROR IMAGES

CHIRALITY AND ENANTIOMERS



Why do we care?

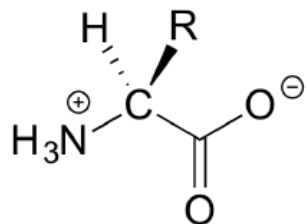
CHIRALITY AND ENANTIOMERS



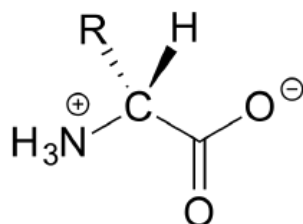
Enantiomers also show **similar chemical properties** until they react with another chiral compound!

Chiral molecules in the human body

Amino acids are chiral!



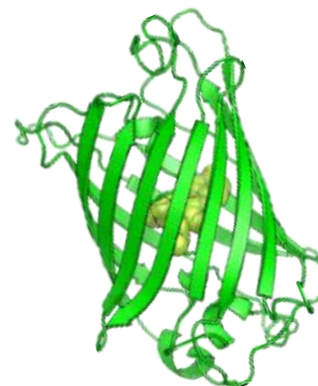
L-amino acids
(common in nature)



D-amino acids
(rare in nature)



Proteins are chiral!



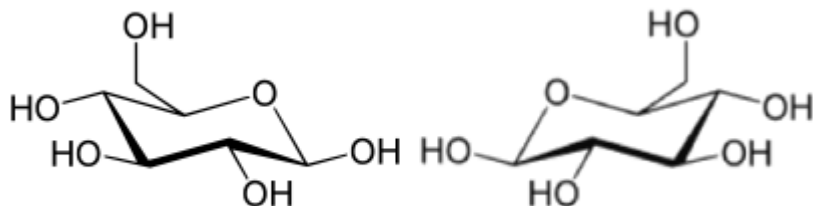
DNA is chiral

Right-handed
helix: **Correct**



Left-handed
helix: **Incorrect**

Carbohydrates (sugars) are chiral!

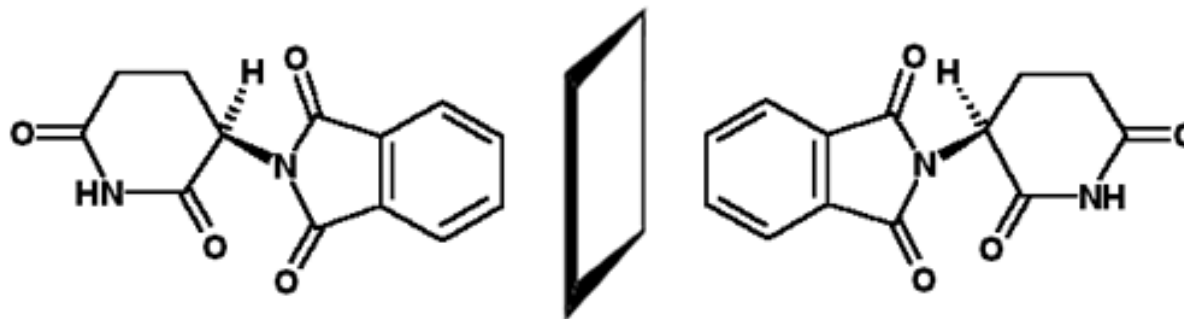


D-Glucose

L-Glucose

Found in nature

Drugs have to (sometimes) be *enantiopure*



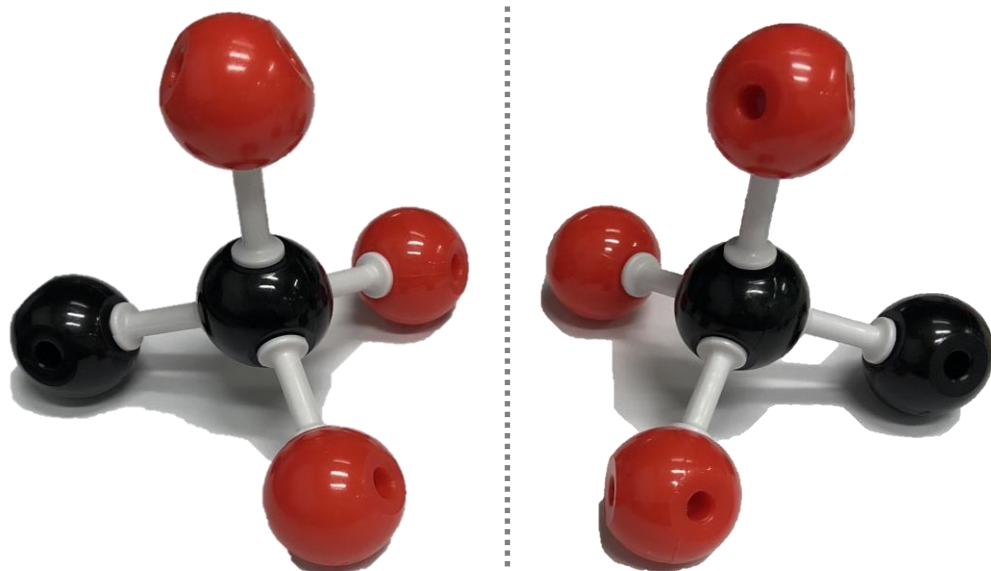
R-Thalidomide
(sleep-inducing)

S-Thalidomide
(teratogenic)

Are these enantiomers?

CHIRAL MOLECULE

1. No plane of symmetry
2. Must have a chiral center- 4 different groups (sp^3 hybridized)



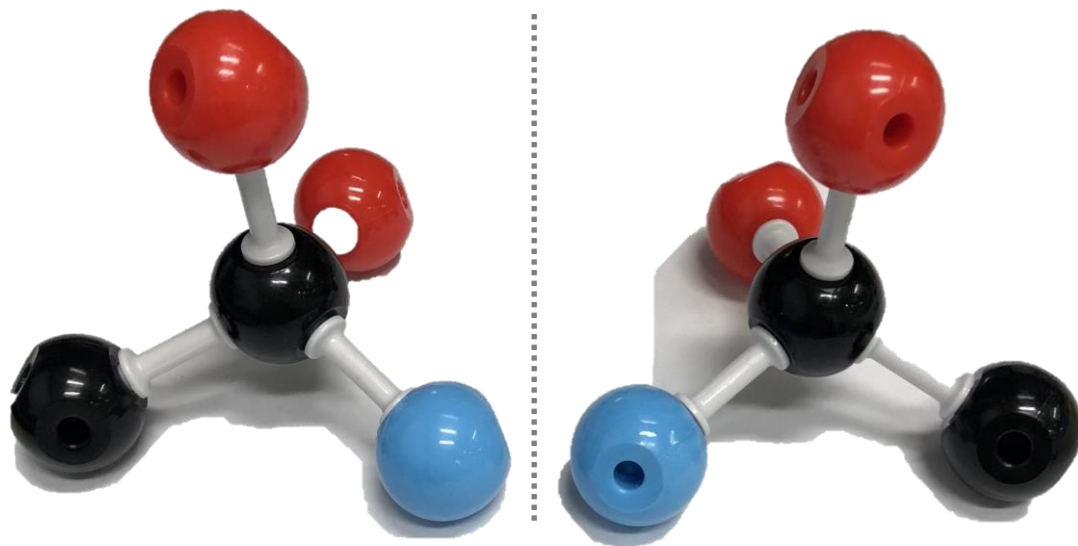
If you flip it, they will line up and look the same!

3 of the same substituent – these are superimposable mirror images - **they are the same molecule; not enantiomers**

Are these enantiomers?

CHIRAL MOLECULE

1. No plane of symmetry
2. Must have a chiral center- 4 different groups (sp^3 hybridized)



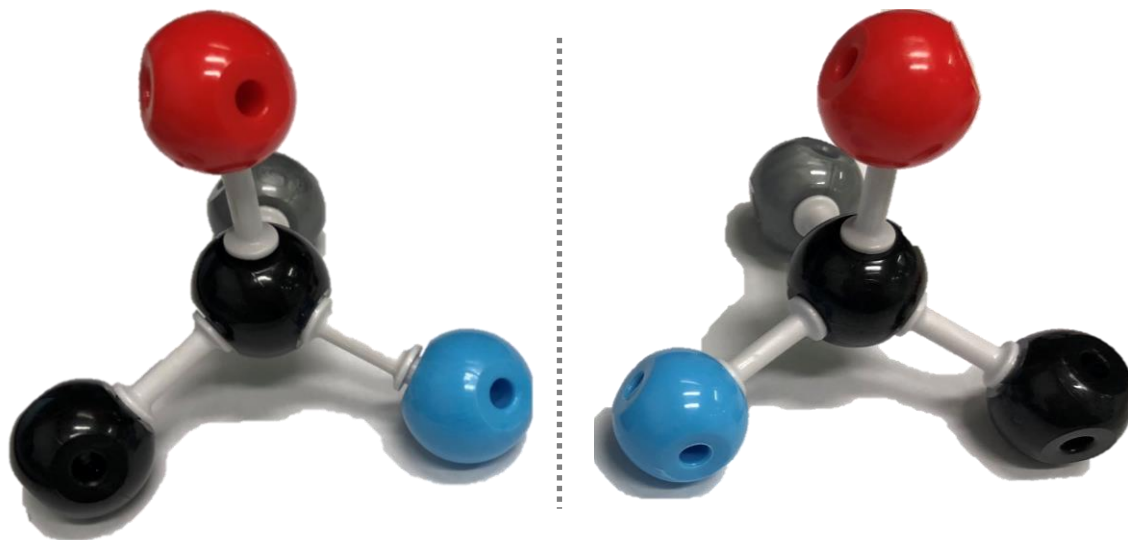
If you flip it, they will line up and look the same!

2 of the same substituent – these are superimposable mirror images - **they are the same molecule; not enantiomers**

Are these enantiomers?

CHIRAL MOLECULE

1. No plane of symmetry
2. Must have a chiral center- 4 different groups (sp^3 hybridized)



All four different substituents – these are nonsuperimposable mirror images – these are enantiomers

Are these enantiomers?

CHIRAL MOLECULE

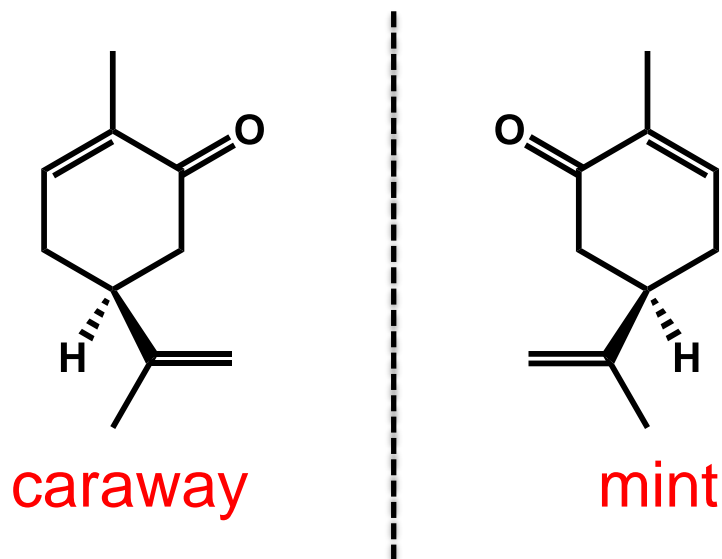
1. No plane of symmetry
2. Must have a chiral center- 4 different groups (sp^3 hybridized)



If you flip it, they do not ever match 😊

All four different substituents – these are nonsuperimposable mirror images – these are enantiomers

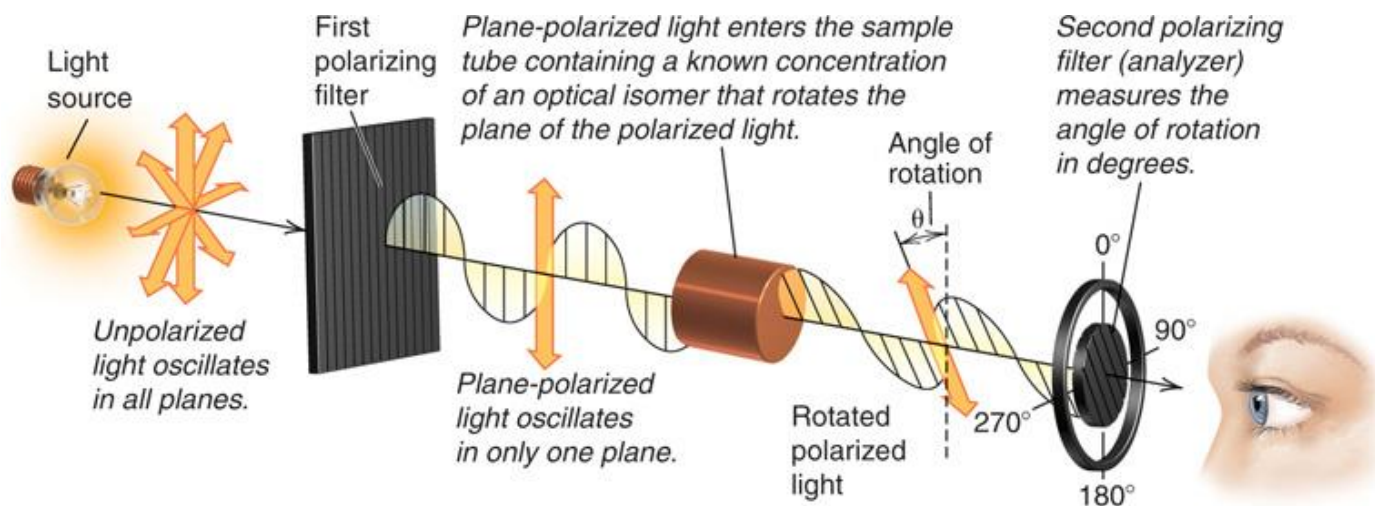
CHIRALITY AND ENANTIOMERS



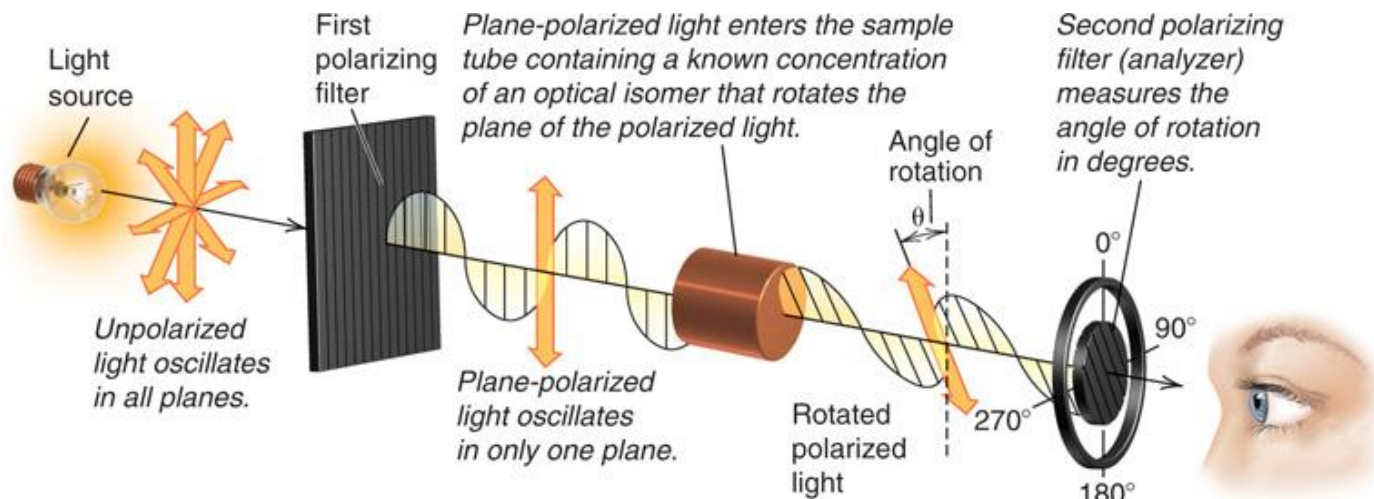
Enantiomers differ in one physical property: chiral molecules are optically active, they can rotate plane polarized light. If a chiral molecule rotates light clockwise, then its mirror image rotates it counterclockwise.

PHYSICAL PROPERTIES OF ENANTIOMERS

Enantiomers differ in one physical property: **they are optically active** i.e. can rotate plane polarized light. If a chiral molecule rotates light clockwise, then its mirror image rotates it counterclockwise to the same extent



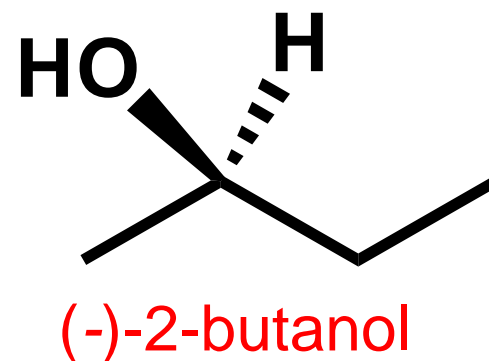
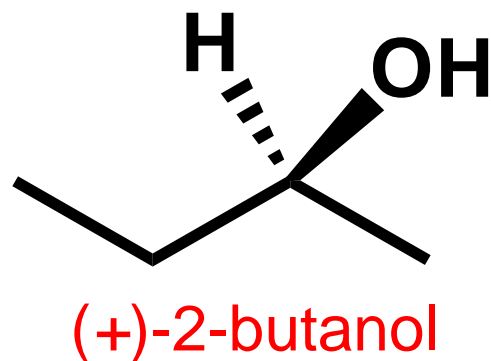
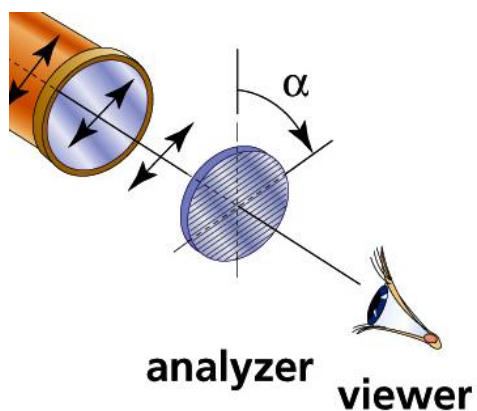
PHYSICAL PROPERTIES OF ENANTIOMERS



Based on optical rotation data: Enantiomers can be classified as **dextrorotatory** or **levorotatory**

Enantiomers are OPTICALLY ACTIVE

RACEMIC MIXTURES

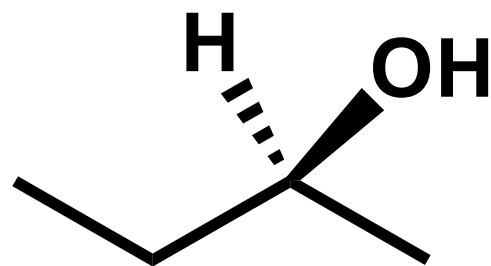
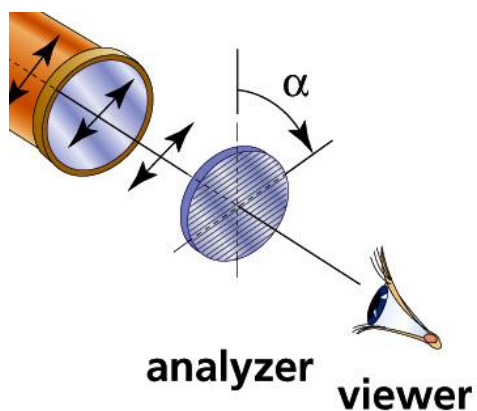


Specific rotation data

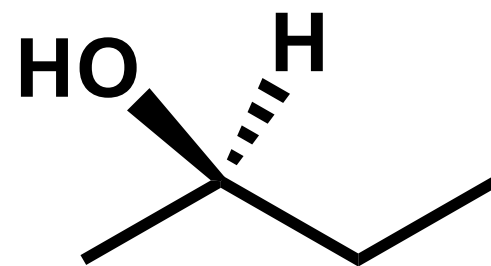
Clockwise rotation
+

Counterclockwise
rotation
-

RACEMIC MIXTURES



(+)-2-butanol



(-)-2-butanol

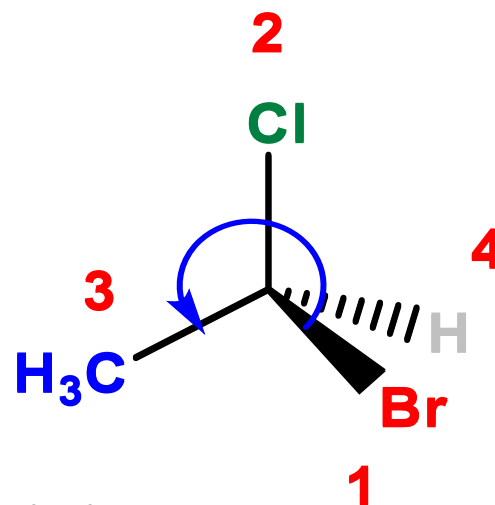
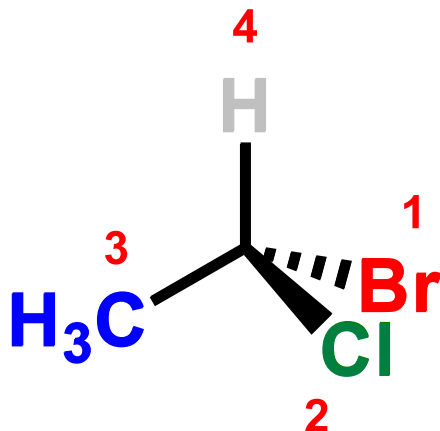
1 : 1 mixture of enantiomers

Racemic Mixture: Optically inactive

Naming Enantiomers: “R” or “S”

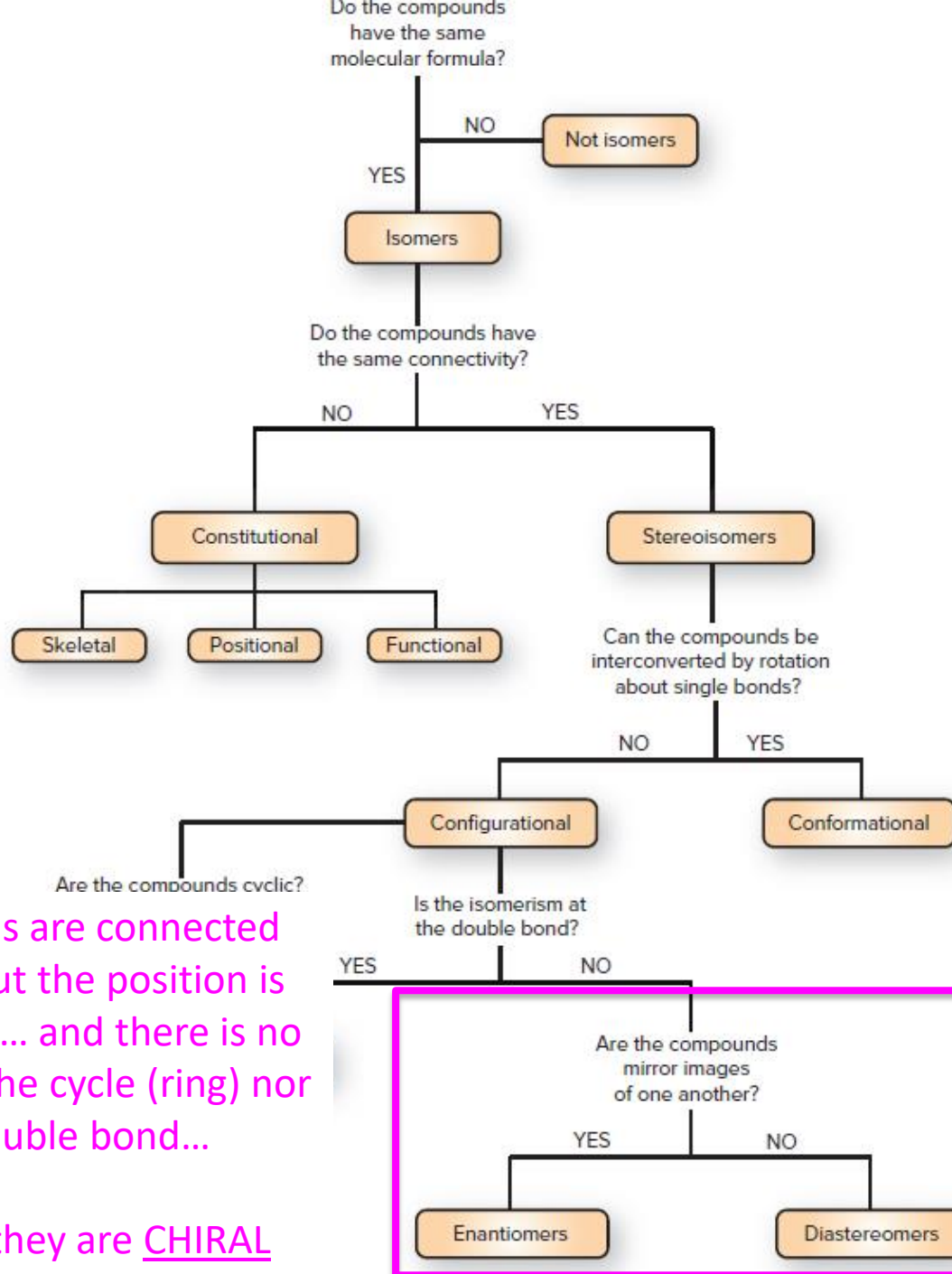
Only for Chiral centres:

1. Assign priority (1:highest to 4:lowest) to all substituents to the chiral center based on atomic number
 2. Point the lowest priority substituent to the back
 3. Draw a curved arrow to show decreasing order of priority (from 1 to 3)- ignore the lowest priority substituent
- “R”: If the curved arrow is drawn clockwise
- “S”: If the curved arrow is drawn counter-clockwise



Counterclockwise - S

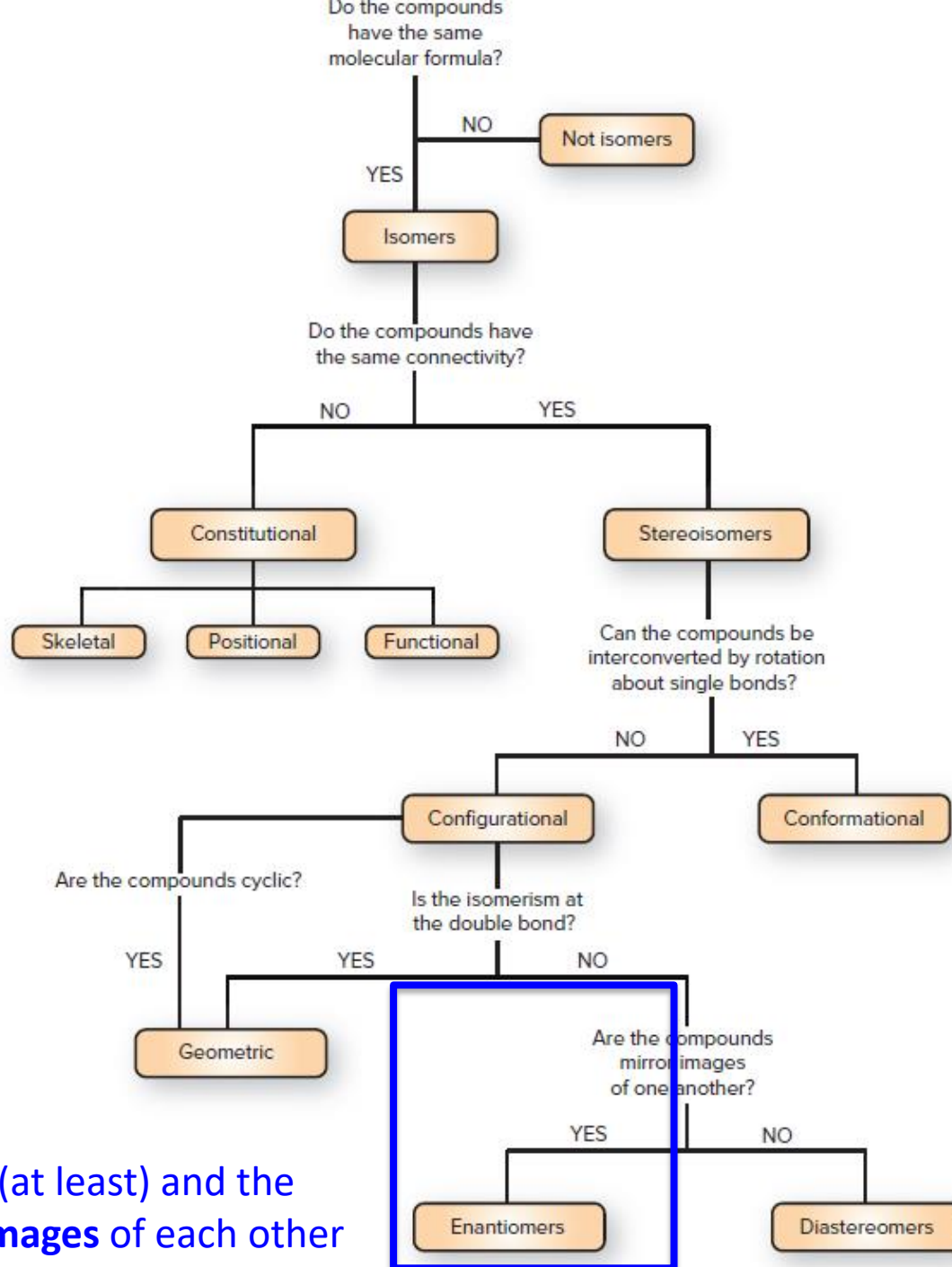
Isomers!



Last case, the atoms are connected in the same way, but the position is somehow different... and there is no isomerism due to the cycle (ring) nor surrounding the double bond...

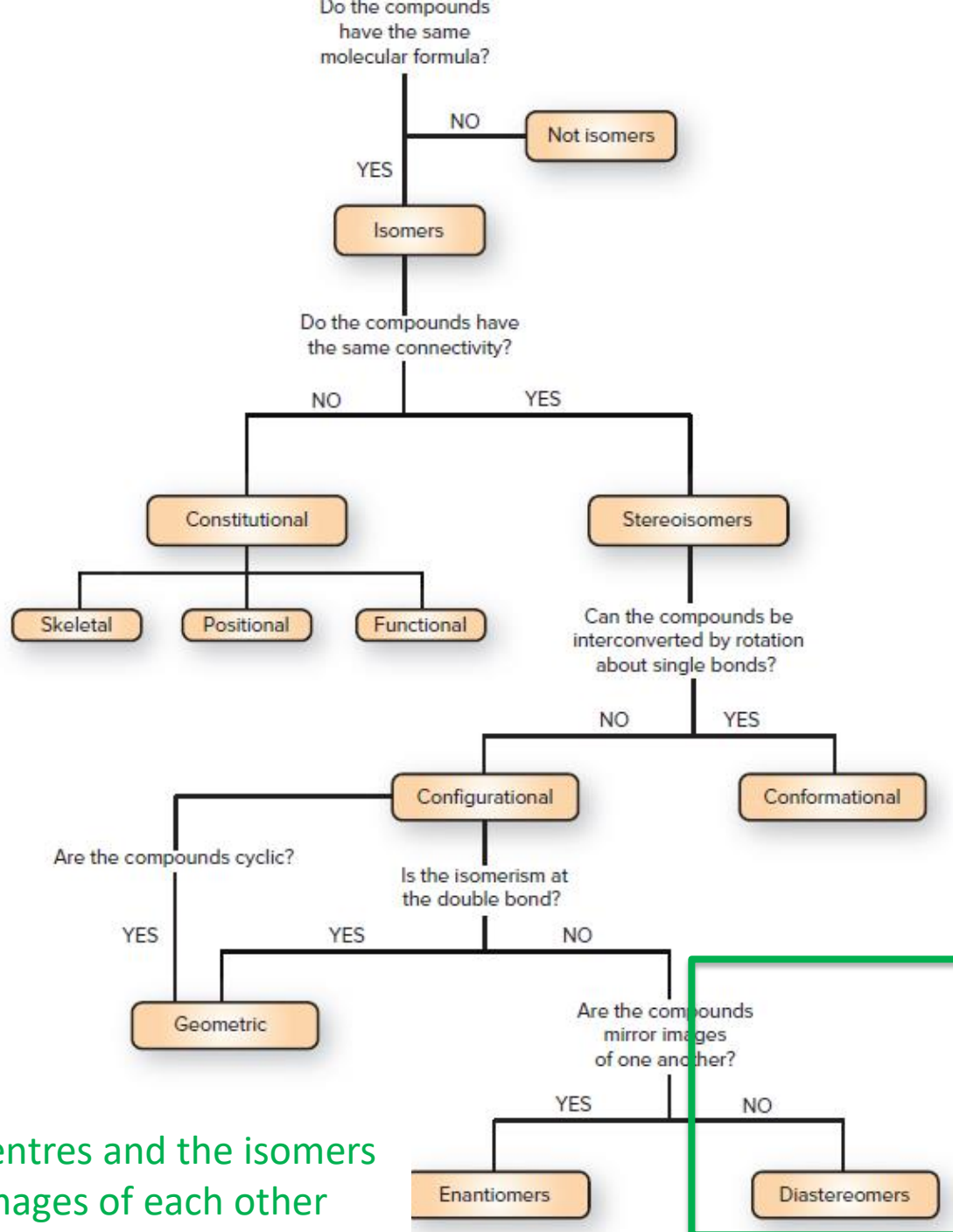
MUST be because they are CHIRAL

Isomers!



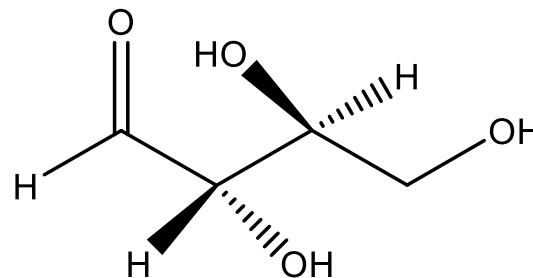
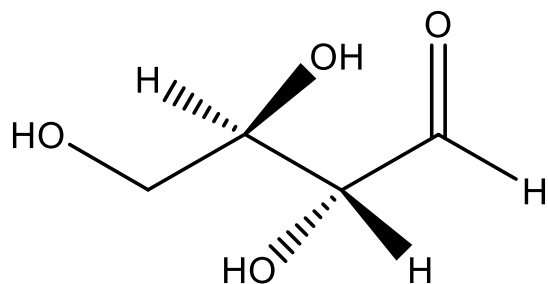
One chiral centre (at least) and the isomers are **mirror images** of each other

Isomers!



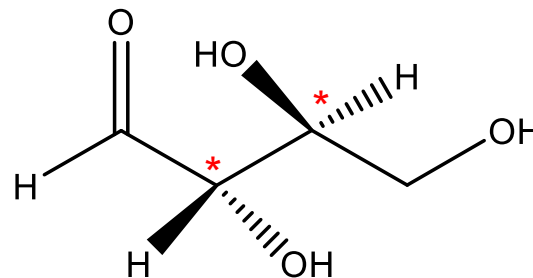
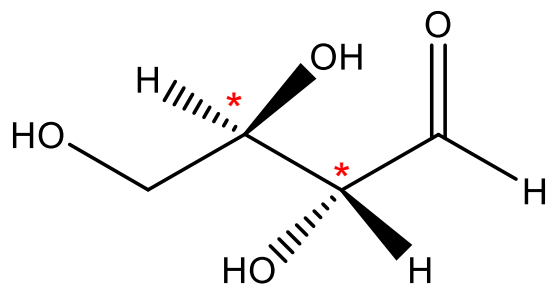
At least two chiral centres and the isomers are **NOT** mirror images of each other

STEREoisomers 3: Diastereomers



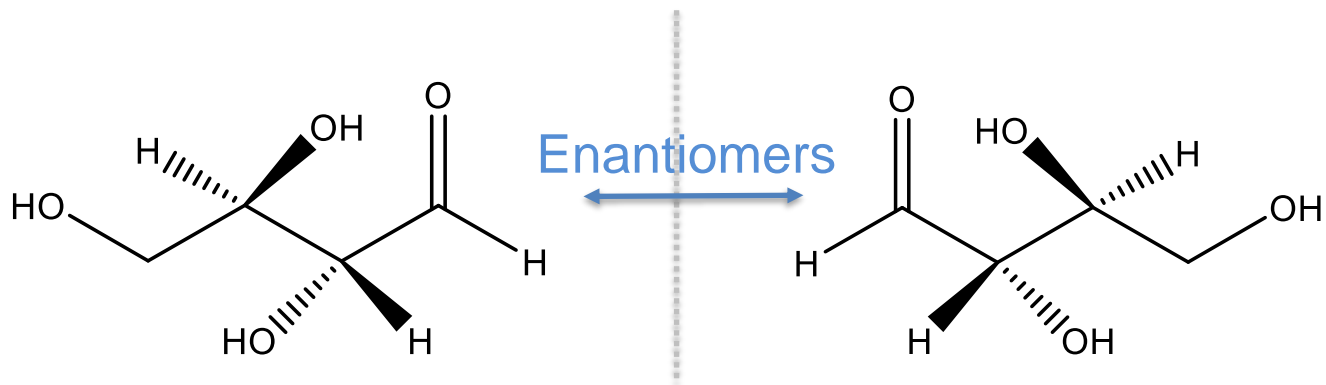
How many chiral carbons does this compound have?

STEREoisomers 3: Diastereomers

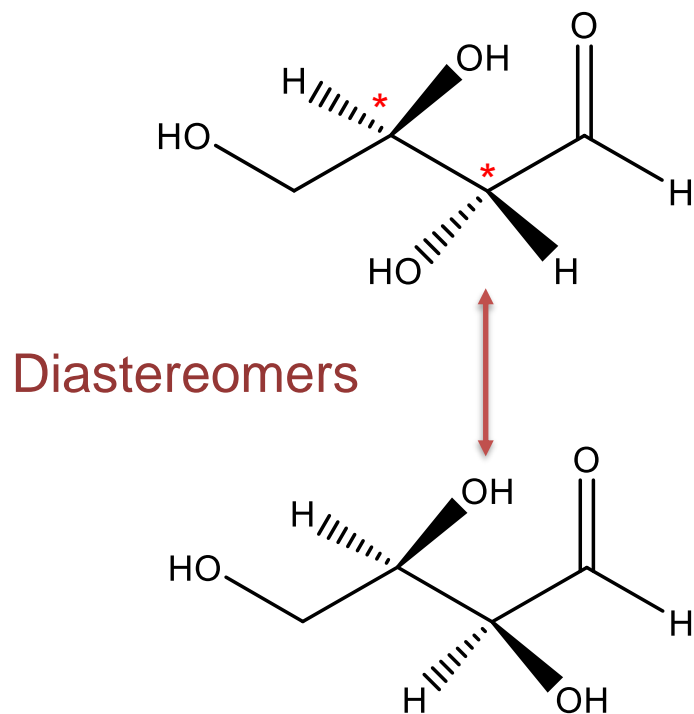


How many chiral carbons does this compound have? 2

STEREISOMERS 3: Diastereomers

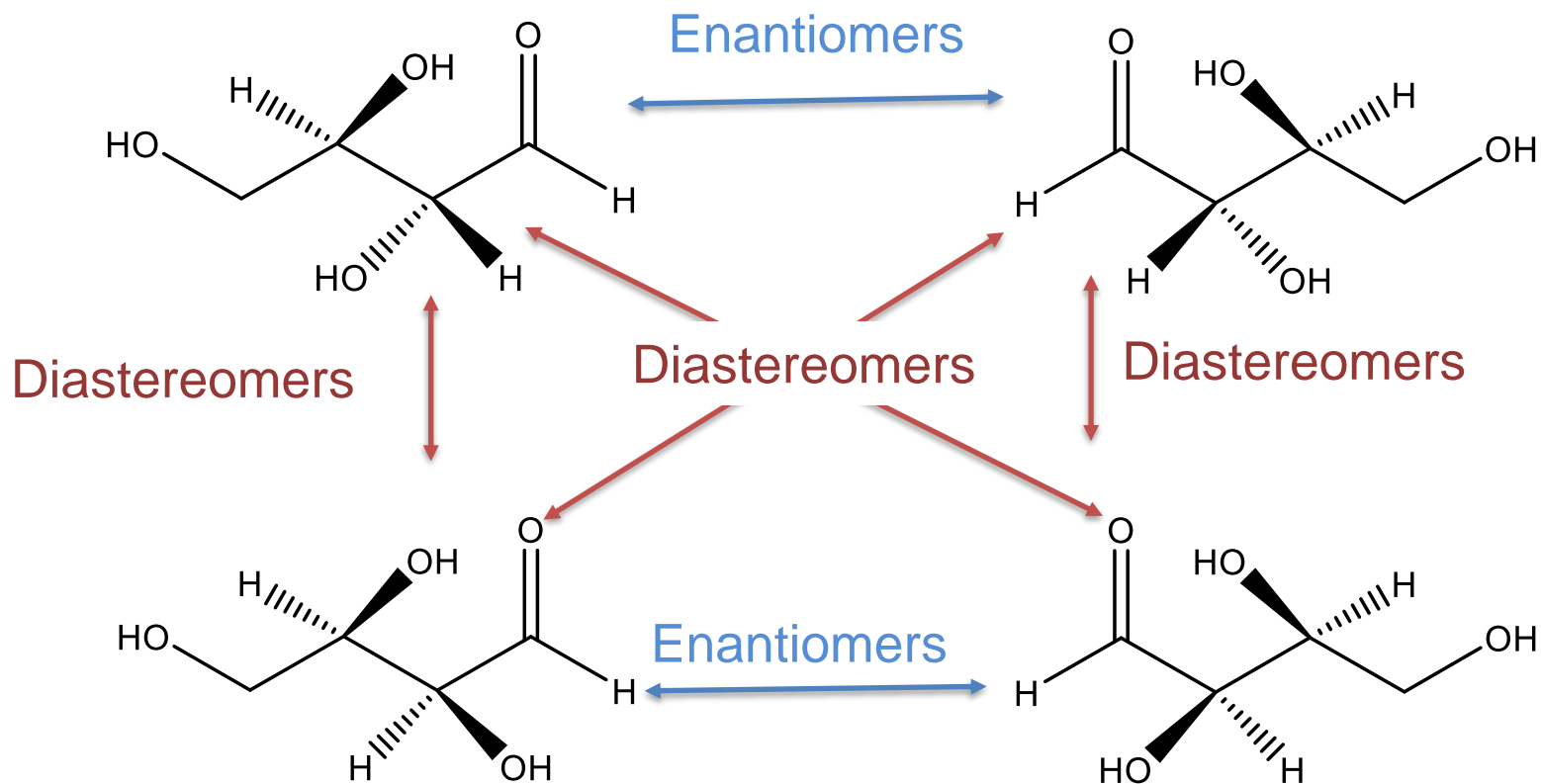


STEREISOISOMERS 3: Diastereomers



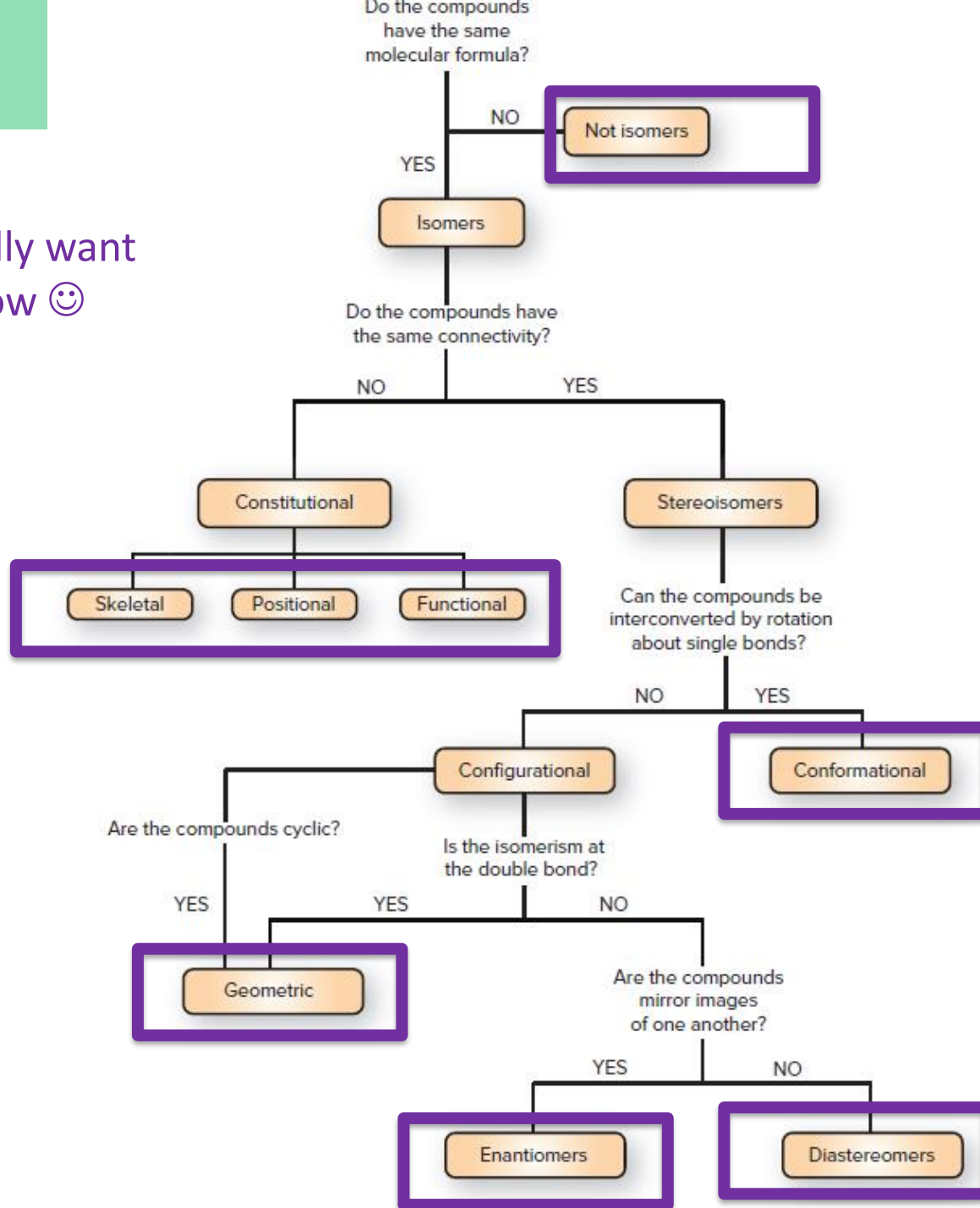
Same chemical formula same bonding **non-mirror images stereoisomers - Diastereomers**

STEREoisomers 3: Diastereomers



Isomers!

What I actually want
you to know 😊



Types of Headache

Migraine



Hypertension



Stress



Organic Chemistry



Congrats you made it!