November 11-15 Notes

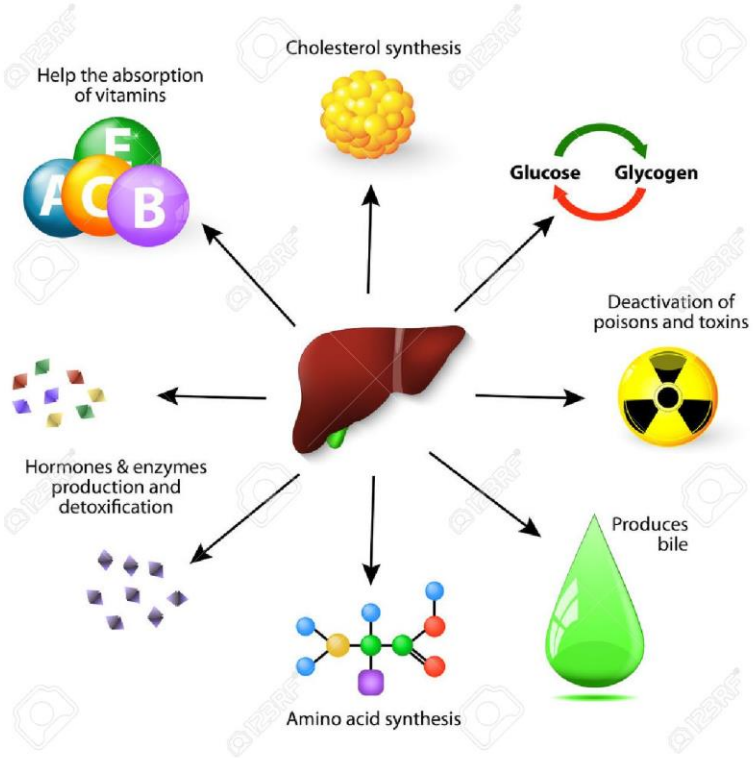
Video 27: Conformation of alkanes

Video 28: Functional groups

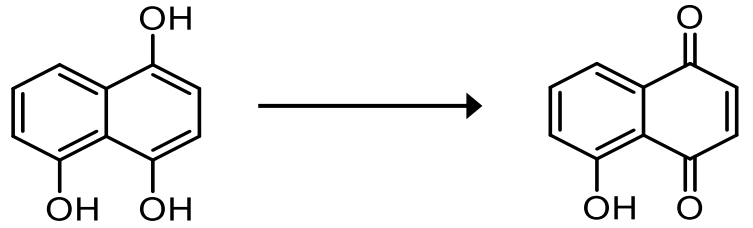
Video 29: Stereochemistry and isomers

Why do we care about organic chemistry?

Understanding chemistry of life around us!



Metabolism

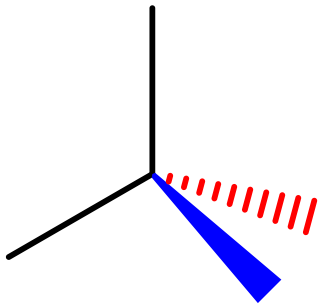


α-hydrojuglone **juglone**

Plant defense

Conformation

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



Solid Line

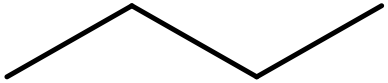
Wedged Bond: bond is pointing forward

Dashed Bond: bond is pointing away

Tetrahedral – sp^3 geometry

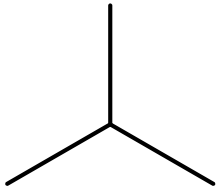
Sawhorse projection

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



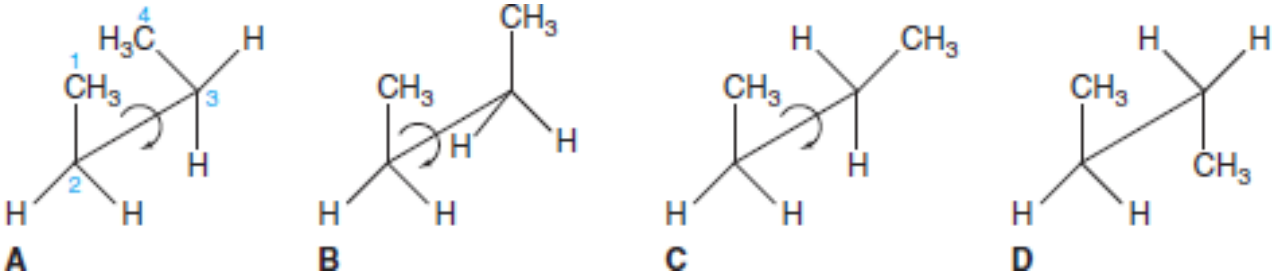
Butane, C_4H_{10}

Butane, C_4H_{10}



2-methylpropane, C_4H_{10}
NOT SAME MOLECULE

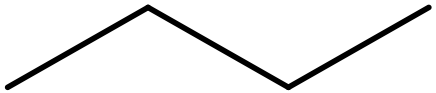
(structural isomer)



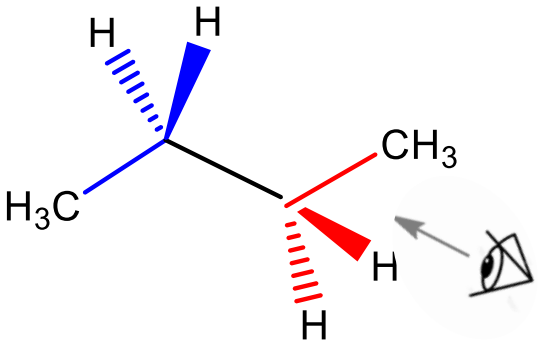
Sawhorse projection of butane --- all the SAME molecule!

Newman Projection

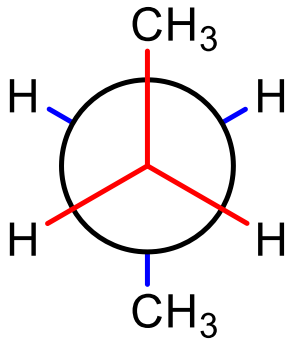
Conformation – The different three-dimensional structures that can be adopted – rotation of atoms about single bonds



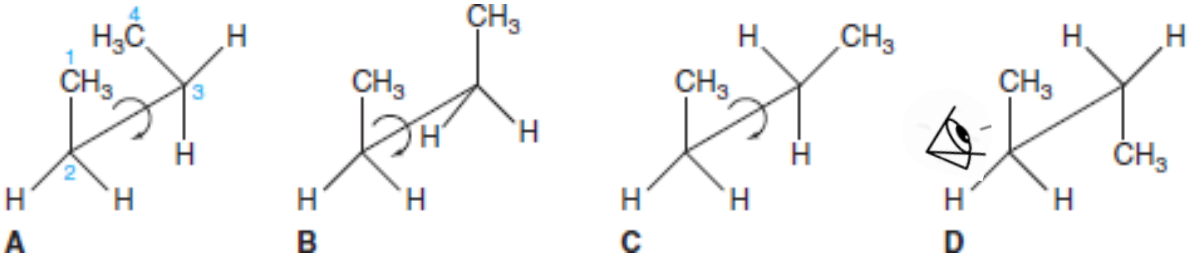
Butane - skeletal



Butane –
showing the conformation

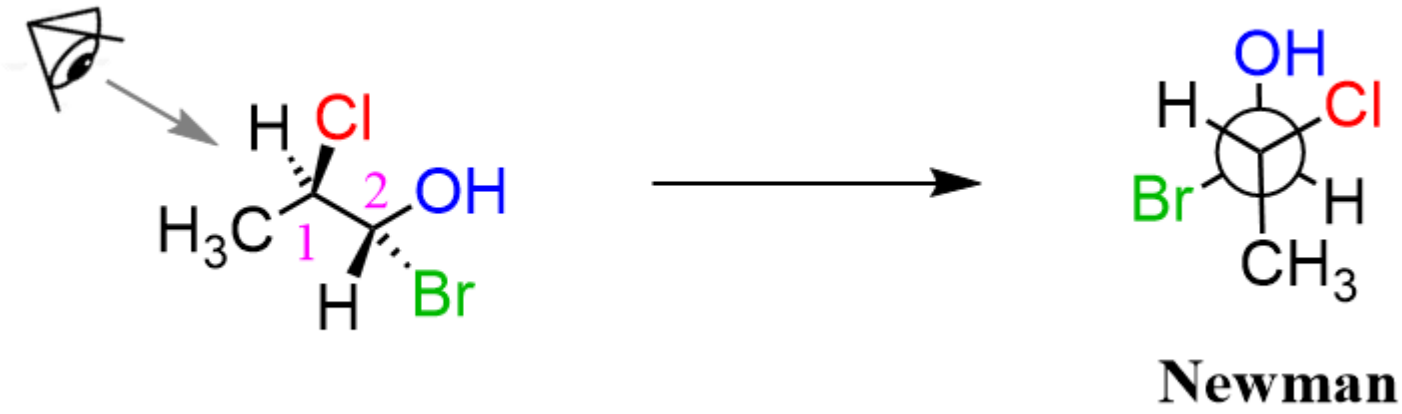


Newman projection of butane

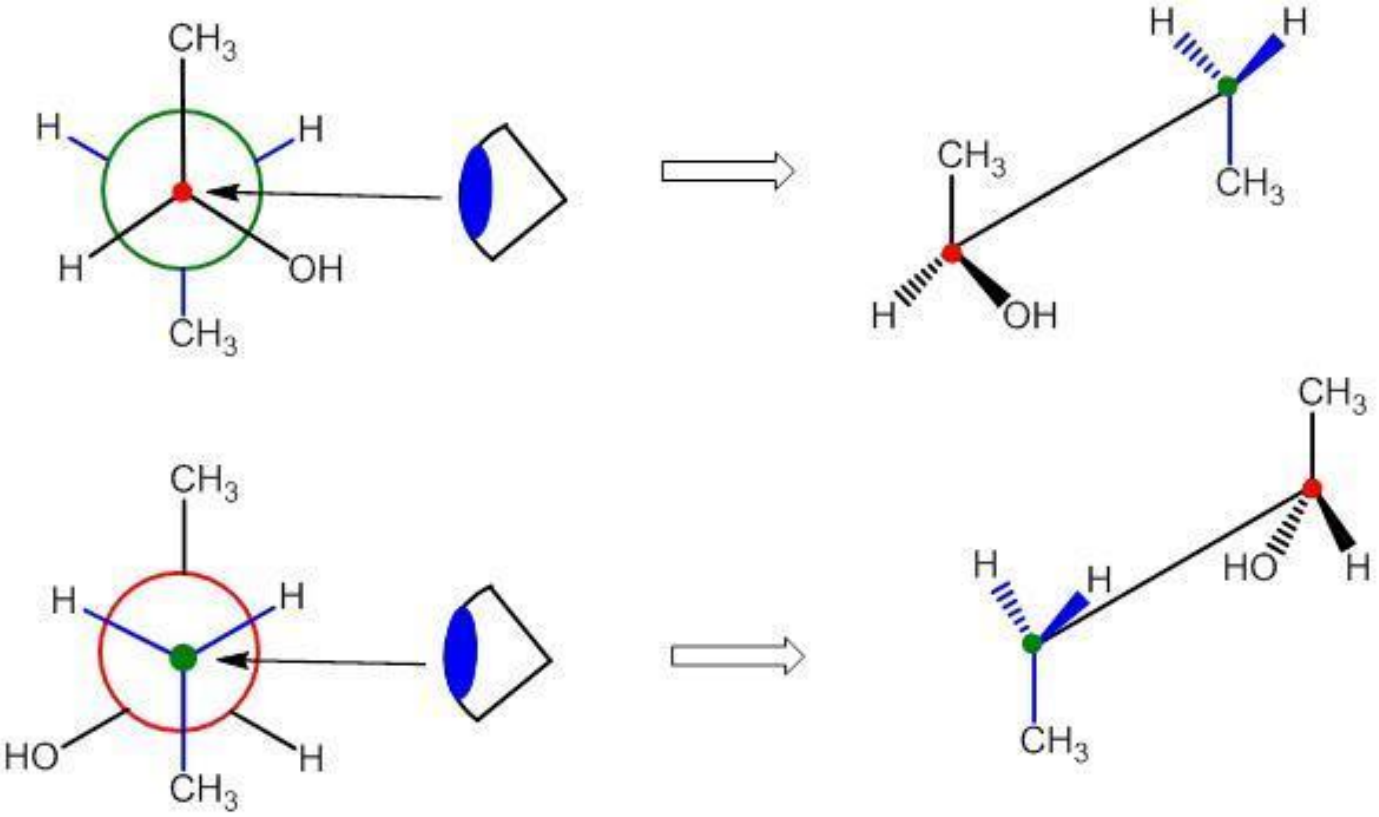


Sawhorse projection of butane

Another Newman Project example

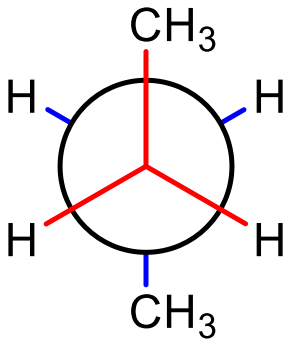


Newman Projection and sawhorse

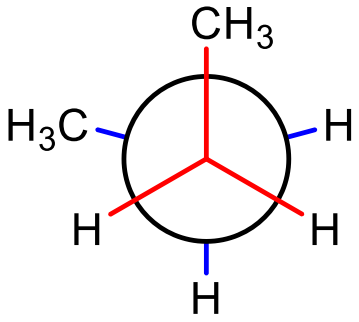


Conformation Changes and Potential Energy

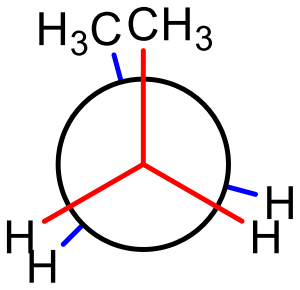
Rotation along the C-C bond:

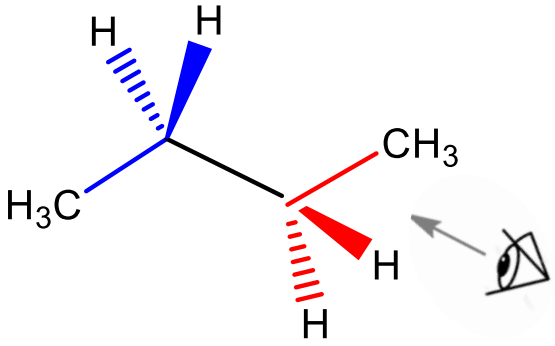


staggered



eclipsed

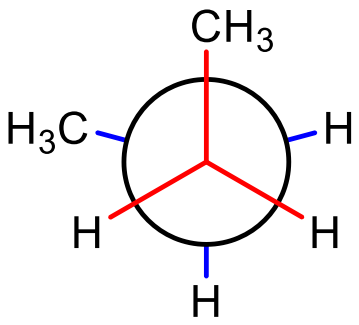




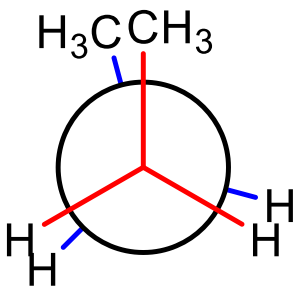
Conformation Changes and Potential Energy

Eclipsed is not stable, it is only a transition state

staggered

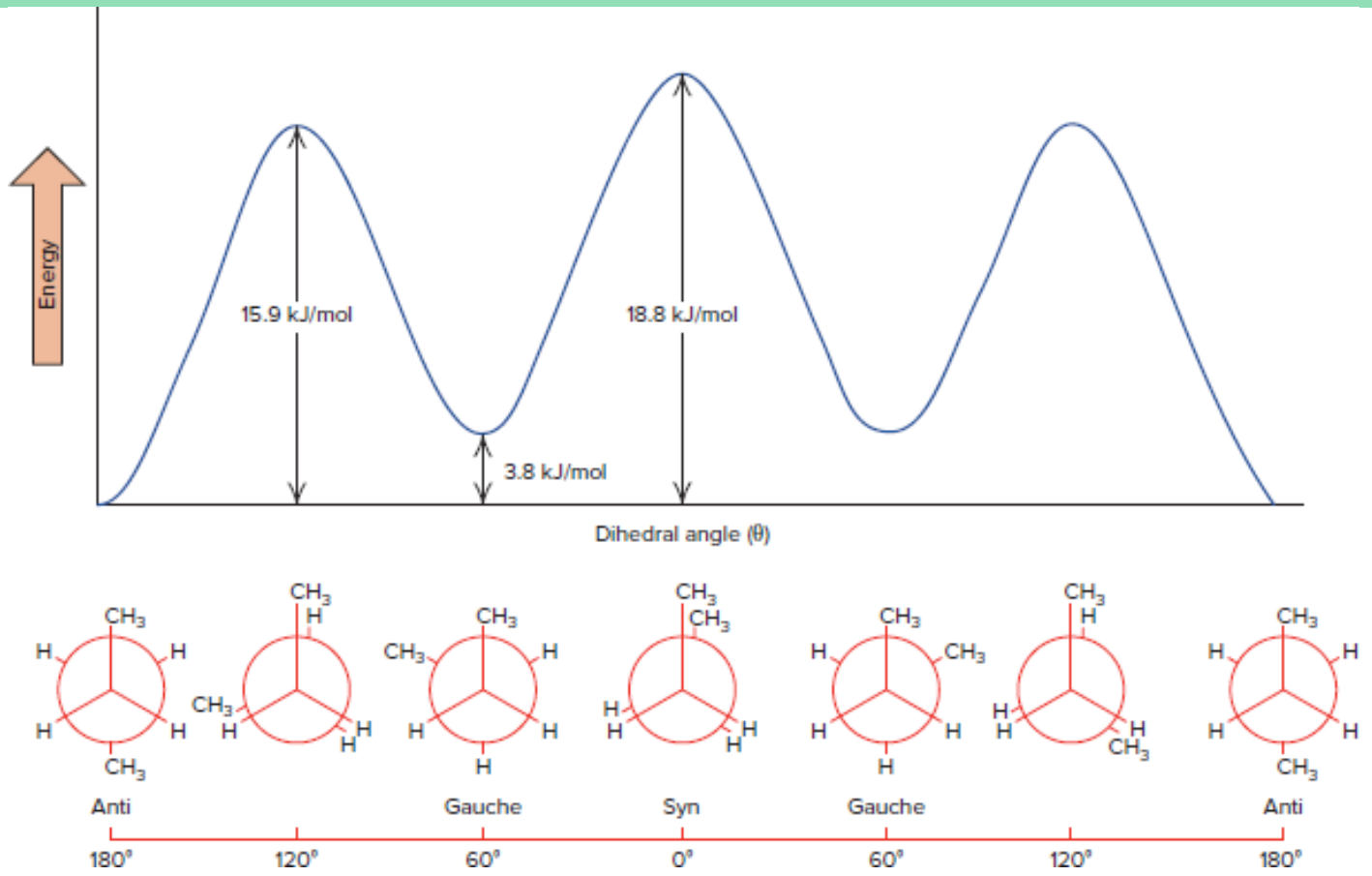


eclipsed



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 CH_3 groups are furthest apart from each other

Extra video to help you visualize

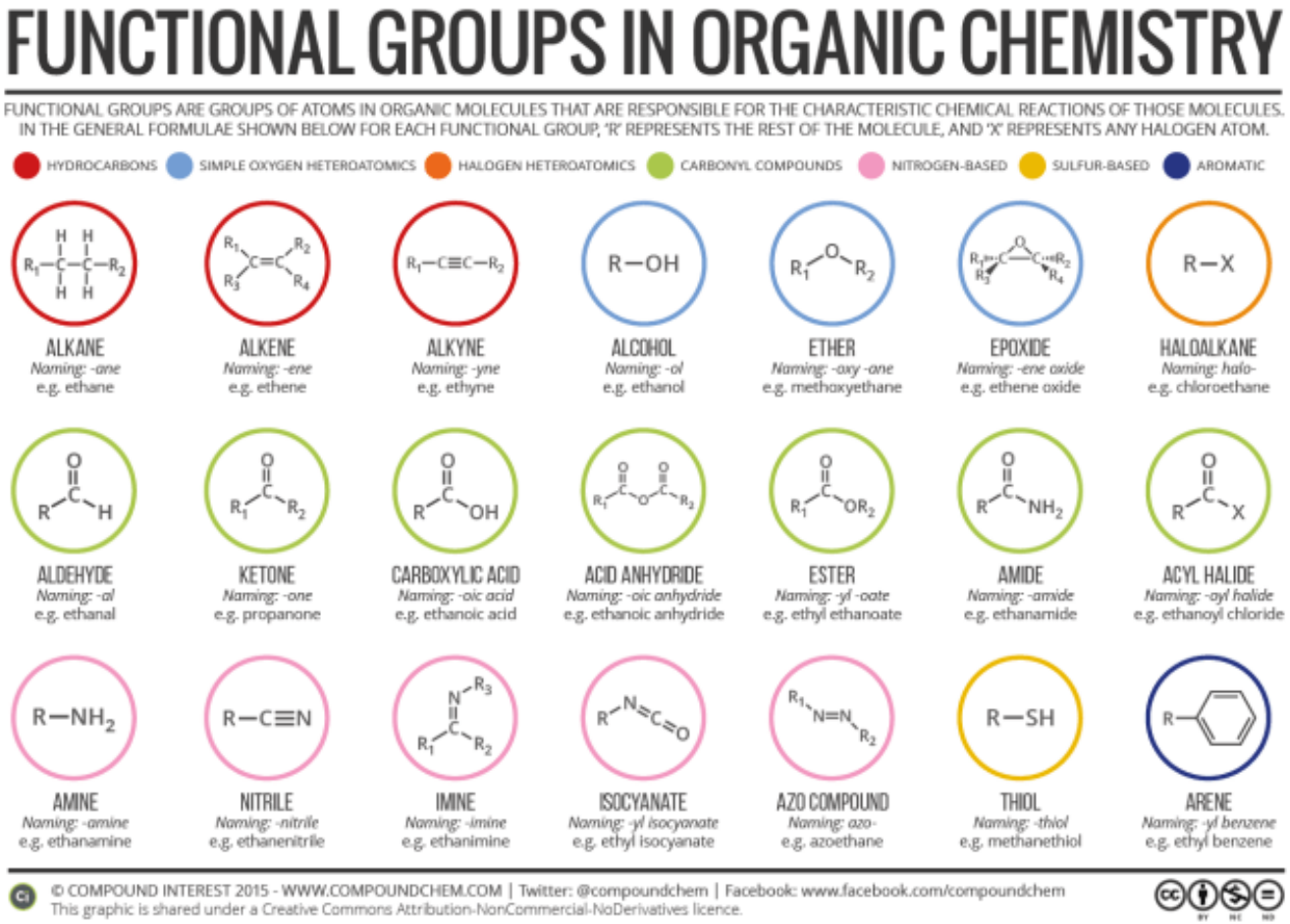
Newman projection:
https://www.youtube.com/watch?v=ETqgo9rAO80

And more on youtube ☺

Nov 11-15

Video 28: Functional groups

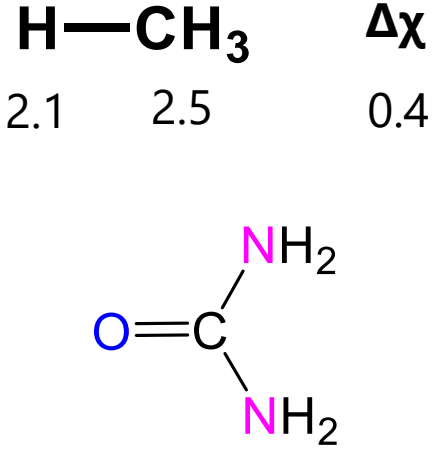
Functional Groups!!!!!!!!!

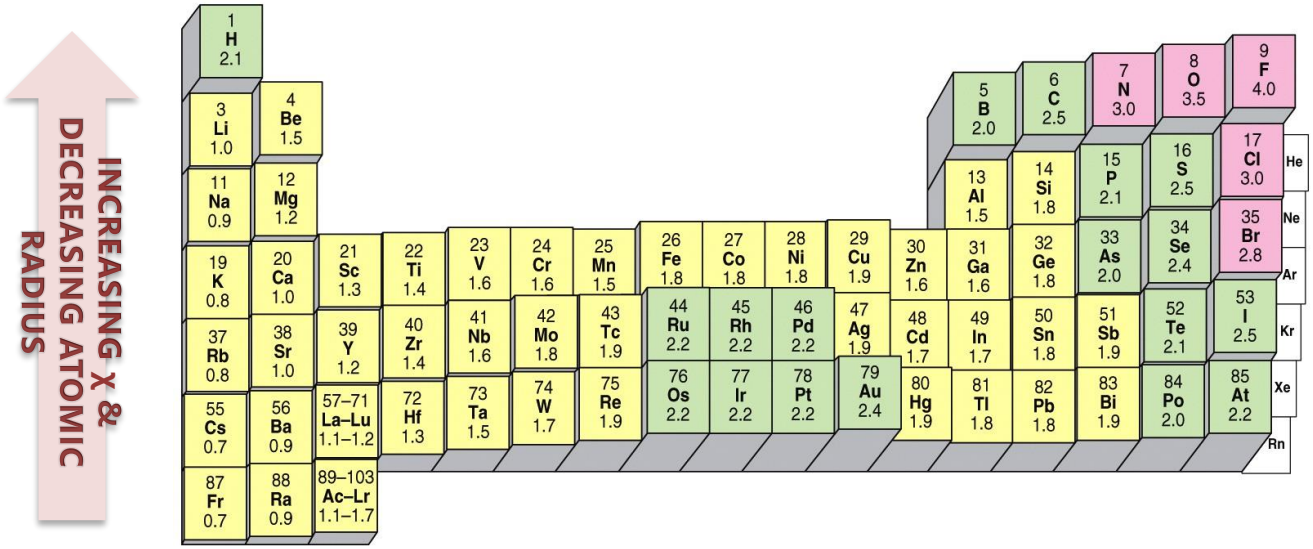


Functional groups = i.e. give the molecule "function"

Hydrocarbons and electronegativity

Electronegativity – ability of an element to attract bonding electrons





Heteroatoms

- Oxygen
- Nitrogen
- Phosphorus
- Sulfur
- Halides

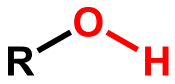
C—F
Δχ
2.5
4.0
1.5

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

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

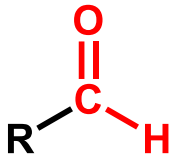
SATURATED

Saturated
Halide

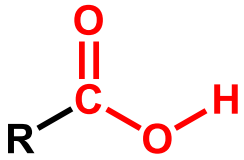


Saturated
Alcohol

UNSATURATED



Unsaturated
Aldehyde



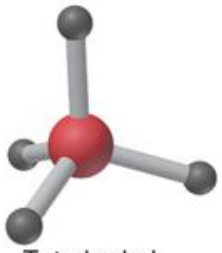
Unsaturated
Carboxylic Acid

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

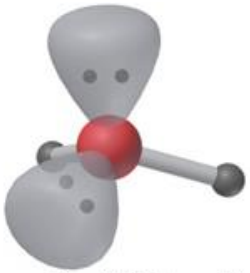
We do this so we focus on the chemistry happening at the functional group (simplify)

Saturated Functional Groups

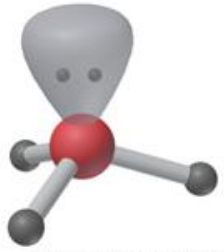
Group	HALO (Halide)	HYDROXYL (Alcohol)	ALKOXY (Ether)	AMINO (Amine)
Functional group	R—X	R–O–H	R–O–R	R–N(R)R



Tetrahedral



Bent (V shaped)



Trigonal pyramidal

Halides:
F
C
I
Br…

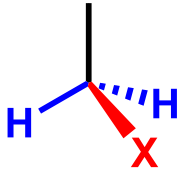
We are focusing on the *functional* group, but it is useful to know the different structural groups involved

Functional Groups: 1. Halides

Saturated Functional Groups

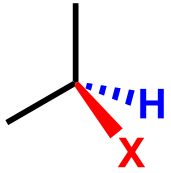
HALO

R—X

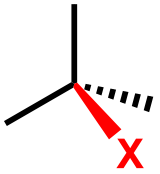


1° halide : Primary Halide
(1° carbon)

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



2° halide: Secondary halide
(2° carbon)



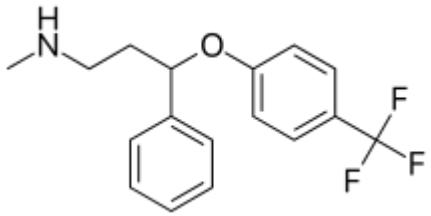
3° halide: Tertiary halide
(3° carbon)

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.

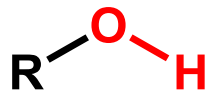


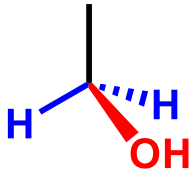
Functional Groups: 2. Alcohols

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

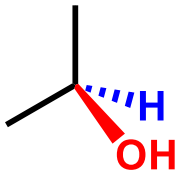
Saturated Functional Groups

HYDROXYL
(Alcohol)



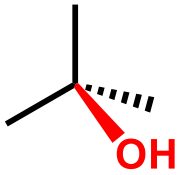


1° alcohol : Primary Alcohol
(1° carbon)



2° alcohol: Secondary Alcohol
(2° carbon)

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

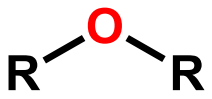


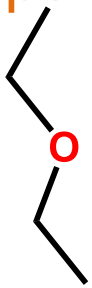
3° alcohol: Tertiary alcohol
(3° carbon)

Functional Groups: 3. Ether

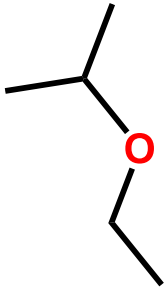
Saturated Functional Groups

ALKOXY
(Ether)





Symmetrical Ether

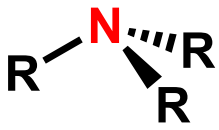


Asymmetrical Ether

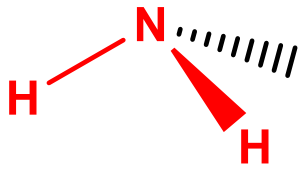
Functional Groups: 4. Amines

Saturated Functional Groups

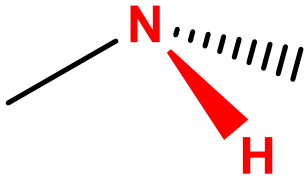
AMINO



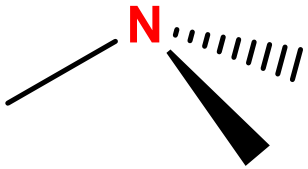
NOTE! NOT based on the carbon at all! Focus on the nitrogen! Based on how many carbons the nitrogen is attached TO. So 1 carbon bonded to the nitrogen = primary; 3 carbons on the nitrogen = tertiary



1° amine : Primary Amine
(1° nitrogen)



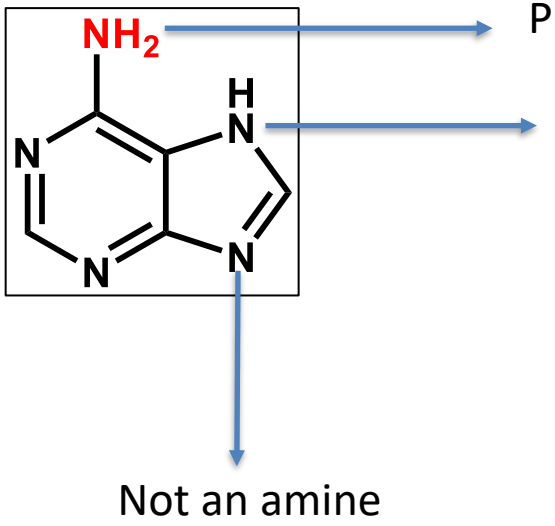
2° amine: Secondary Amine
(2° nitrogen)



3° amine: Tertiary amine
(3° nitrogen)

Saturated Functional Groups

Nitrogens with a double bond are NOT amino groups!



Primary amine

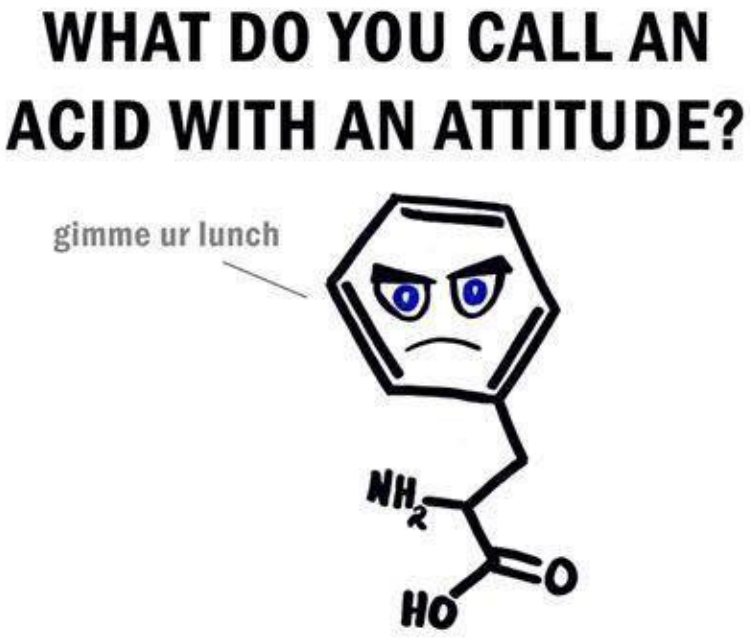
Not an amine

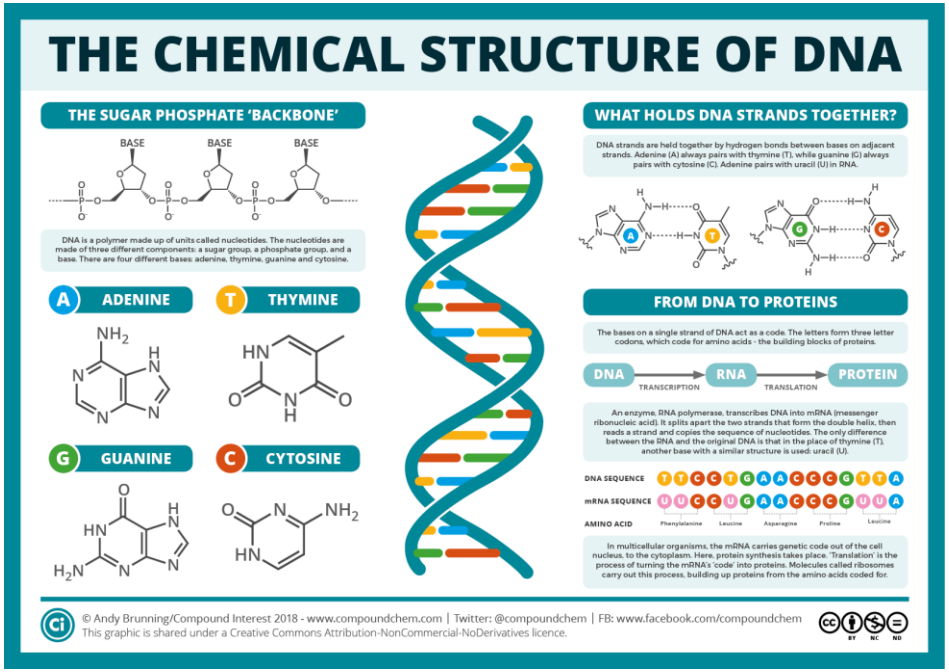
This one is tricky (due to resonance)

Not an amine

Functional Groups: 4. Amines

Amines are super important!

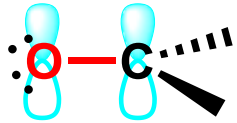


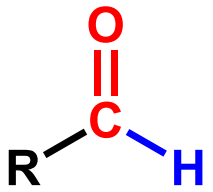


Functional Groups

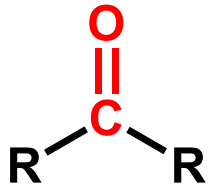
Unsaturated Functional Groups

CARBO**NYL**





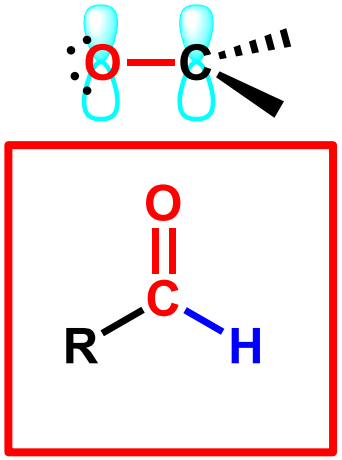
aldehyde



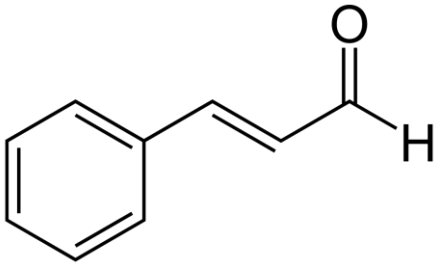
ketone

Functional Groups: 5. Aldehyde

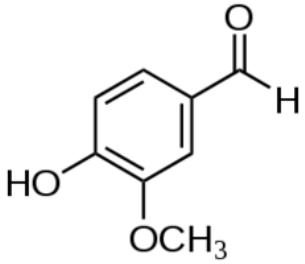
Unsaturated Functional Groups



Aldehyde: RCHO



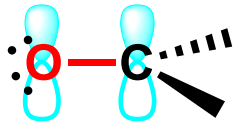
Cinnamaldehyde

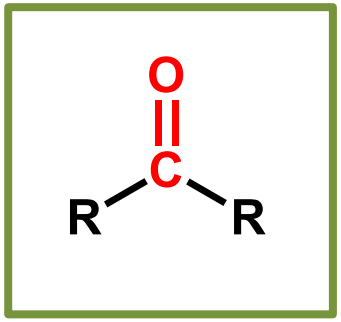


Vanillin

Functional Groups: 6. Ketone

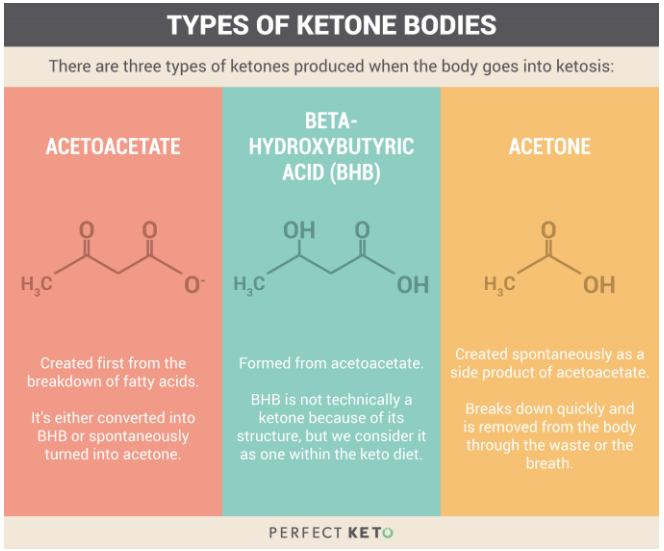
Unsaturated Functional Groups





Ketone: RCOR

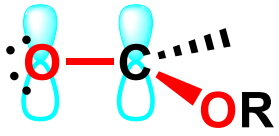
Ketosis

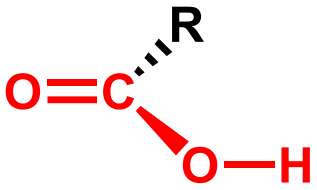


Functional Groups

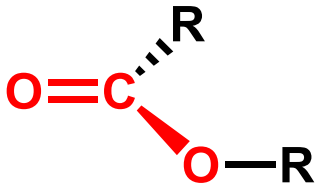
Unsaturated Functional Groups

CARBO**XYL**





Carboxylic acid

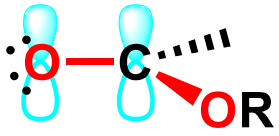


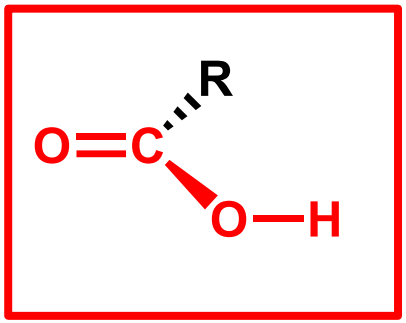
ester

Functional Groups: 7. Carboxylic Acid

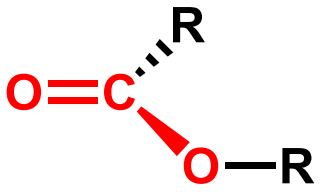
Unsaturated Functional Groups

CARBO**XYL**





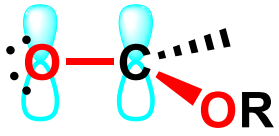
Carboxylic Acid: RCOOH

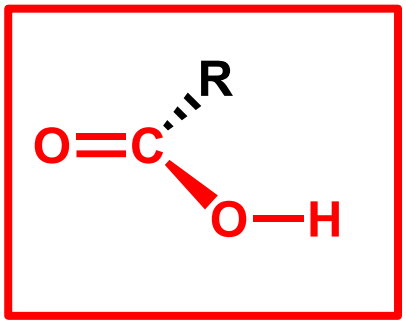


Functional Groups: 8. Ester

Unsaturated Functional Groups

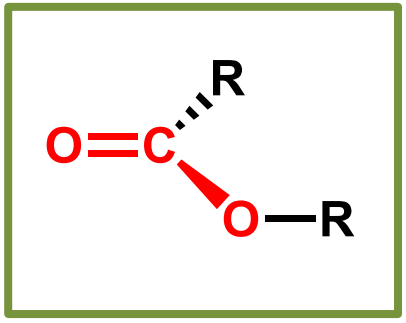
CARBO**XYL**





Carboxylic Acid: RCO_2H

Acetic acid
(ethanoic acid)



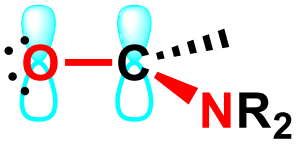
Ester: RC(O)OR

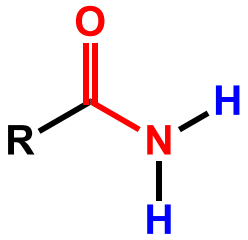
Examples:
-fruity smells
-see page 916

Functional Groups: 9. Amide

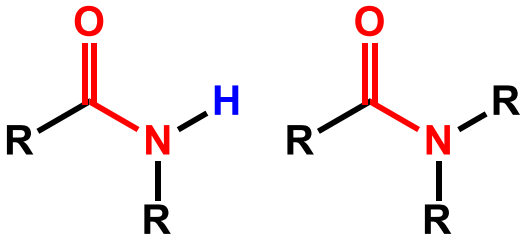
Unsaturated Functional Groups

AMIDO





unsubstituted amides



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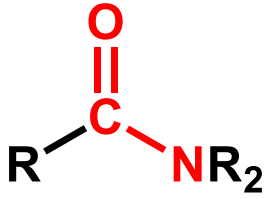
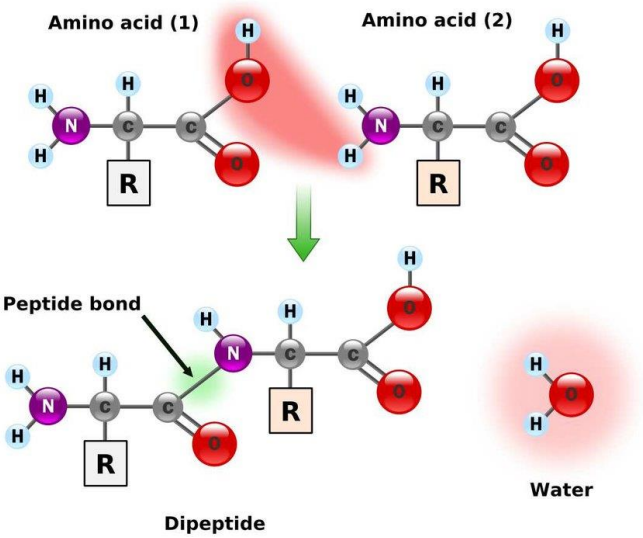


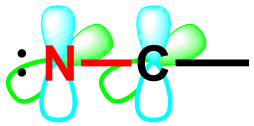
Amides: $RCONR_2$



Functional Groups: 10. Nitriles

Unsaturated Functional Groups

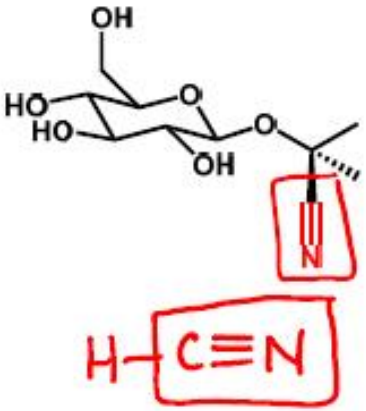
CYANO

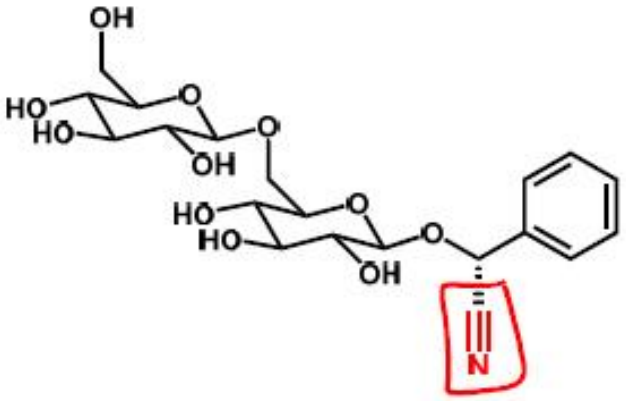


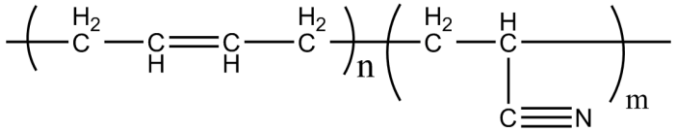
N≡C—R

Nitrile

RCN

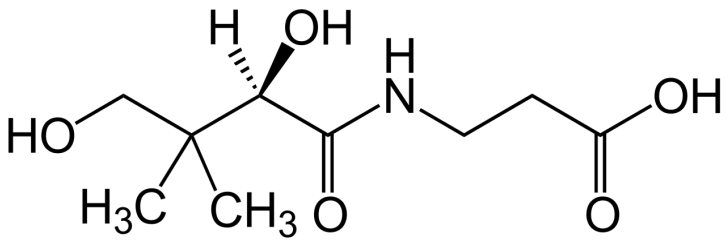




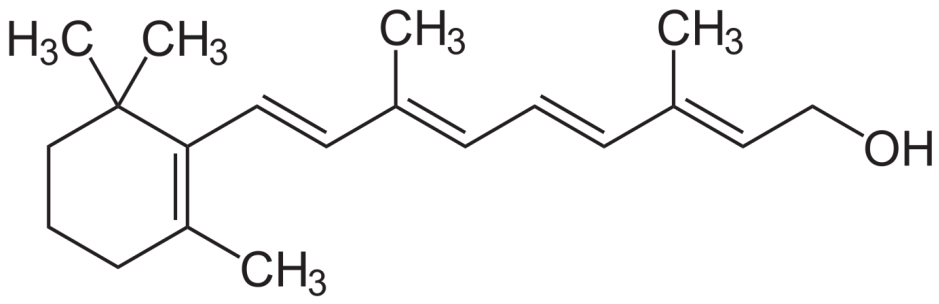


Functional Groups in Biological Compounds: PRACTICE

Circle and name the functional groups



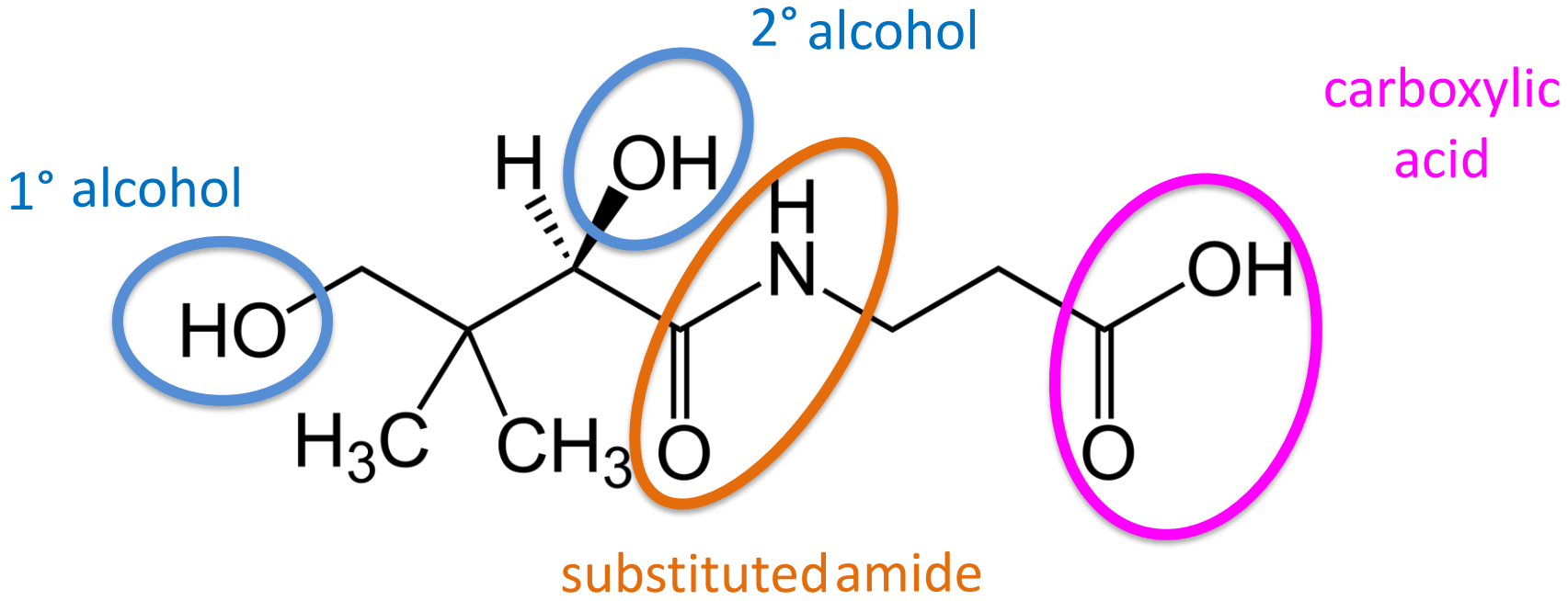
Vitamin B5
(pantothenic acid)



Vitamin A1
(retinol)

Functional Groups in Biological Compounds: PRACTICE

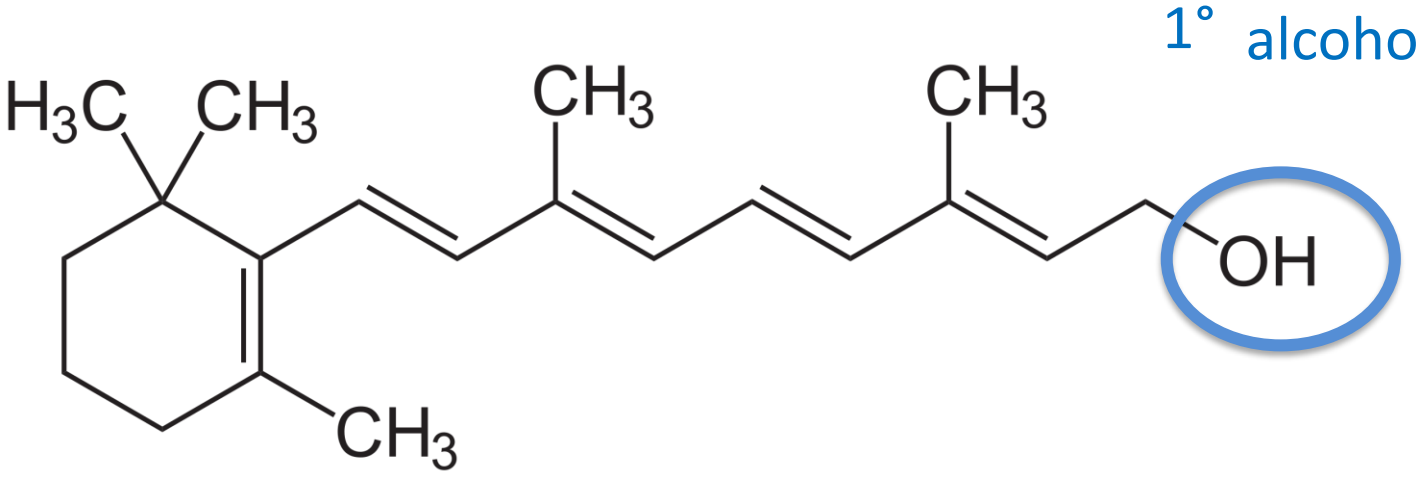
Circle and name the functional groups



Vitamin B5
(pantothenic acid)

Functional Groups in Biological Compounds: PRACTICE

Circle and name the functional groups



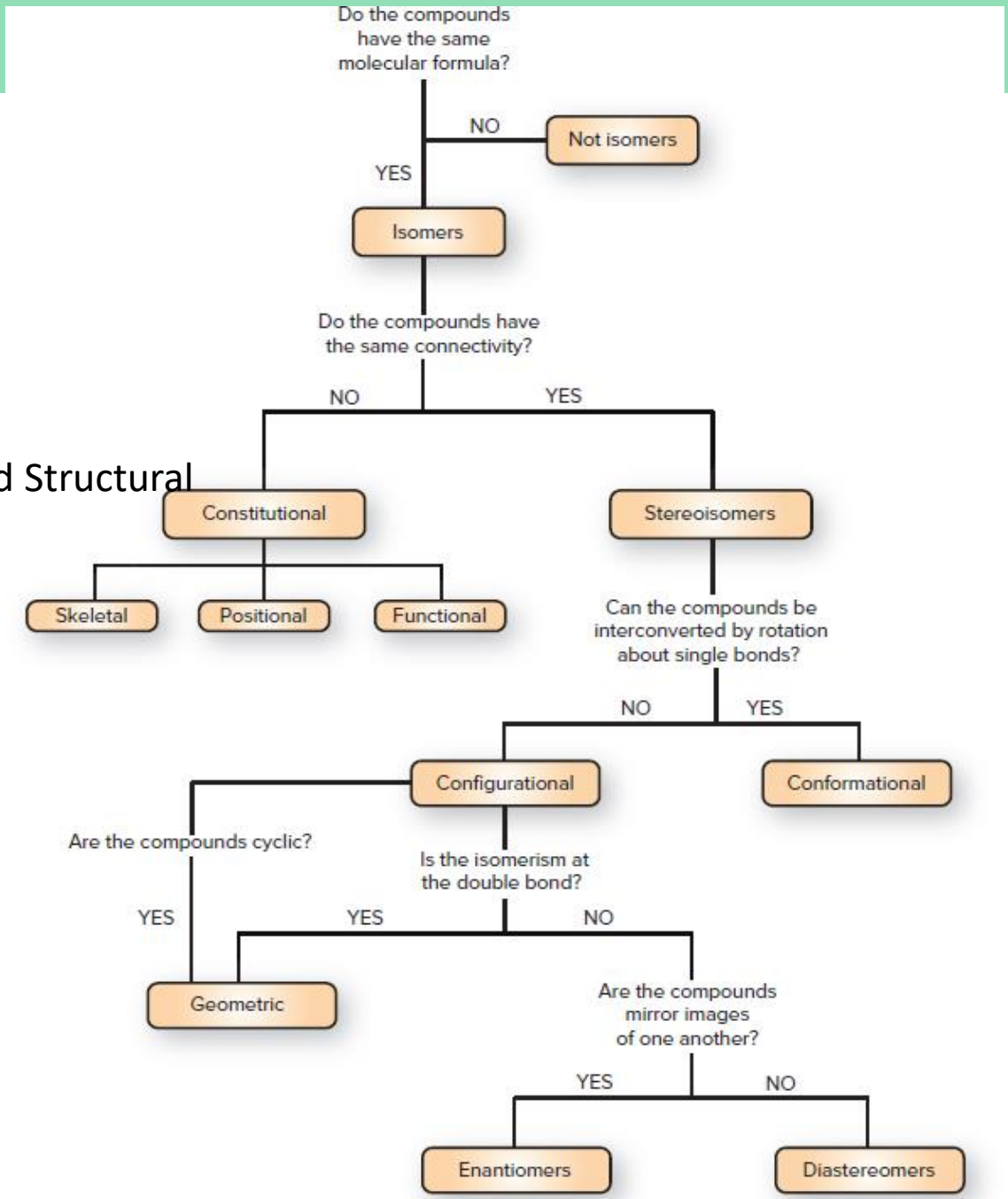
Vitamin A1
(retinol)

November 13-17

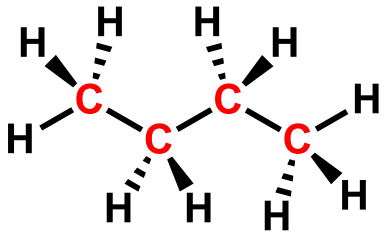
Video 29: Stereochemistry and isomers

Isomers!

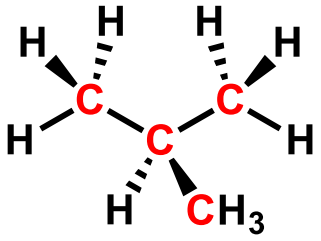
also called Structural



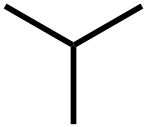
Different kinds of structural isomers



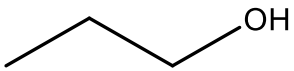
BUTANE

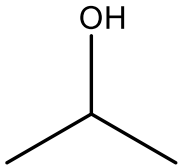


ISOBUTANE

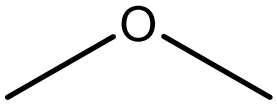


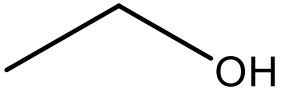
Same chemical formula different arrangement of carbon atoms – SKELETAL ISOMERS





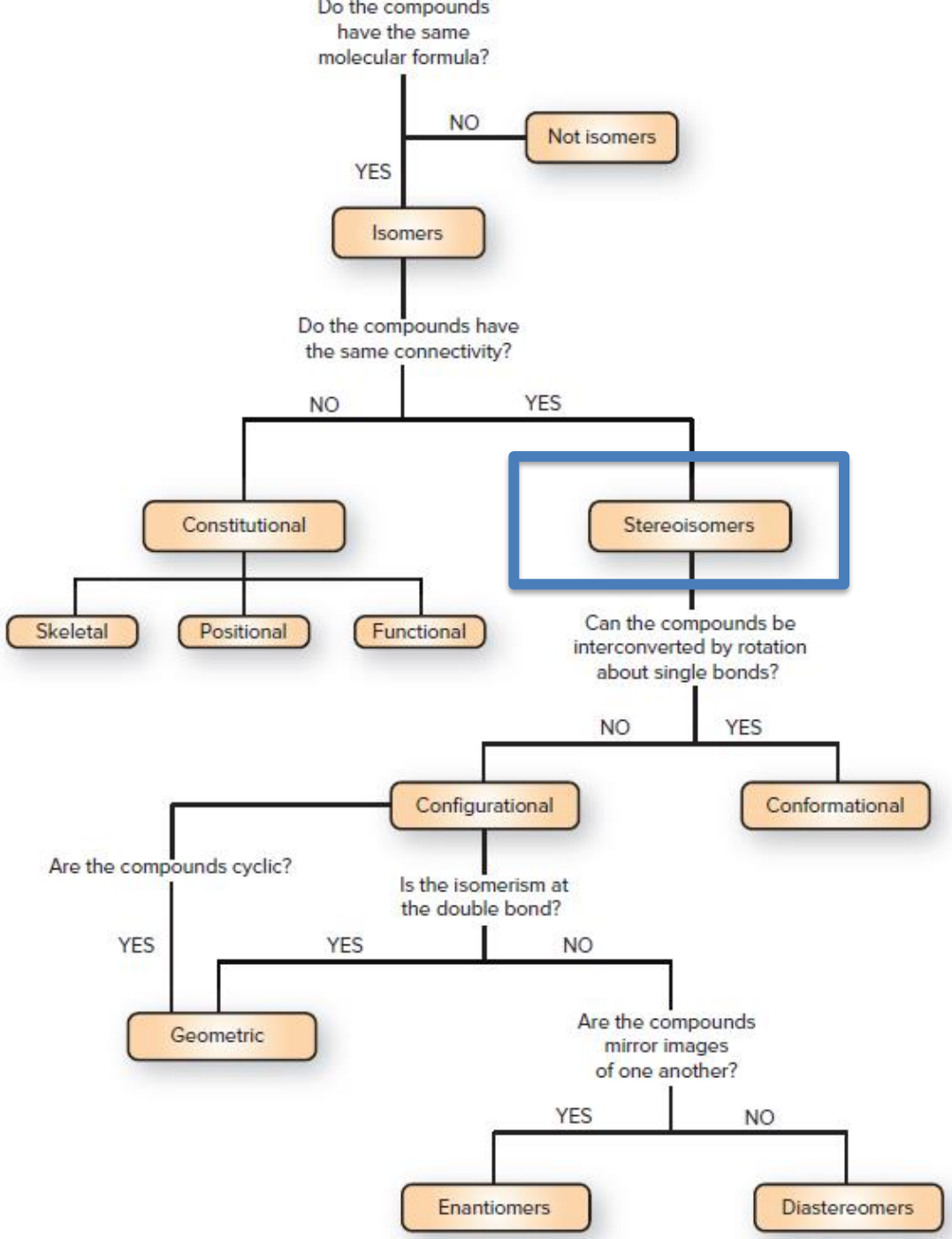
Same chemical formula different position of functional group – POSITIONAL ISOMERS





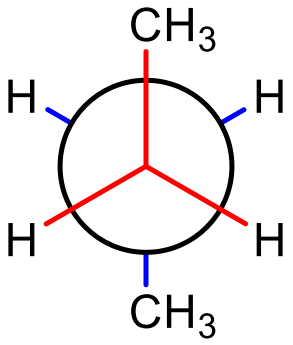
Same chemical formula different functional groups – FUNCTIONAL ISOMERS

Isomers!

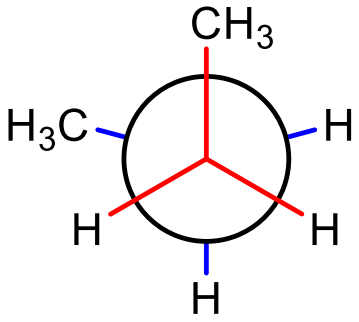

Do the compounds have the same molecular formula?
NO
Not isomers
YES
Isomers
Do the compounds have the same connectivity?
NO
YES
Constitutional
Stereoisomers
Skeletal
Positional
Functional
Can the compounds be interconverted by rotation about single bonds?
NO
YES
Configurational
Conformational
Are the compounds cyclic?
Is the isomerism at the double bond?
YES
YES
NO
Geometric
Are the compounds mirror images of one another?
YES
NO
Enantiomers
Diastereomers

Conformation Changes and Potential Energy

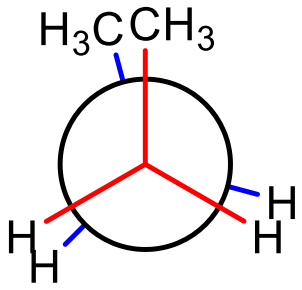
Reminder these are all *conformational* isomers of each other (really just the same molecule in different conformation)

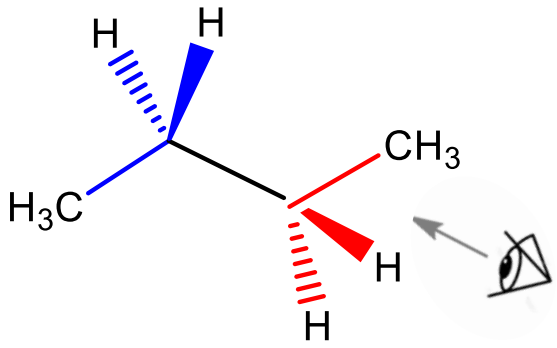


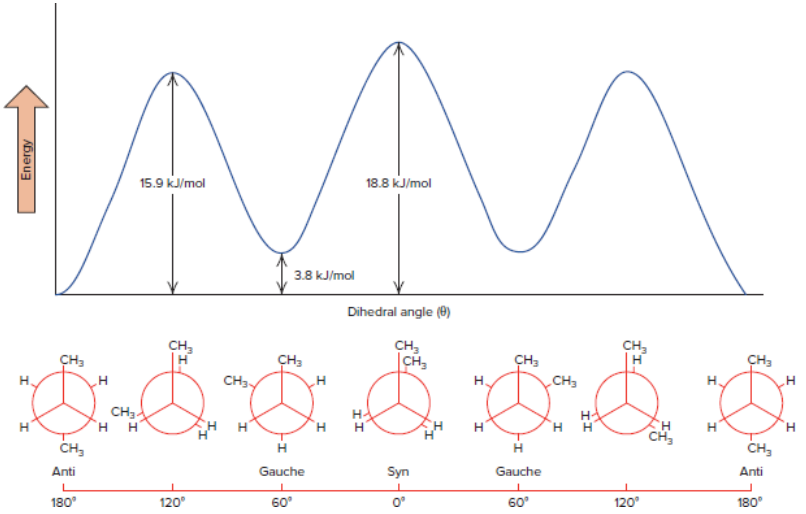
staggered



eclipsed

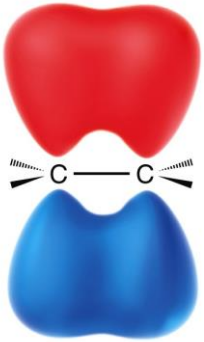


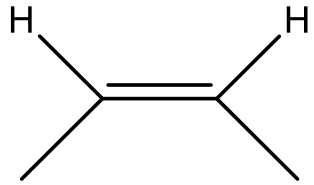


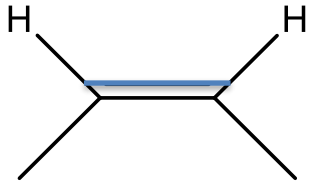


Conformation Changes in Alkanes

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



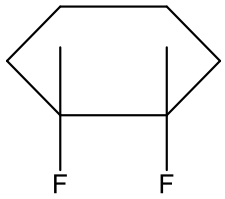


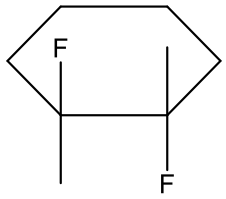


Cannot rotate!
Because of
double bond!

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

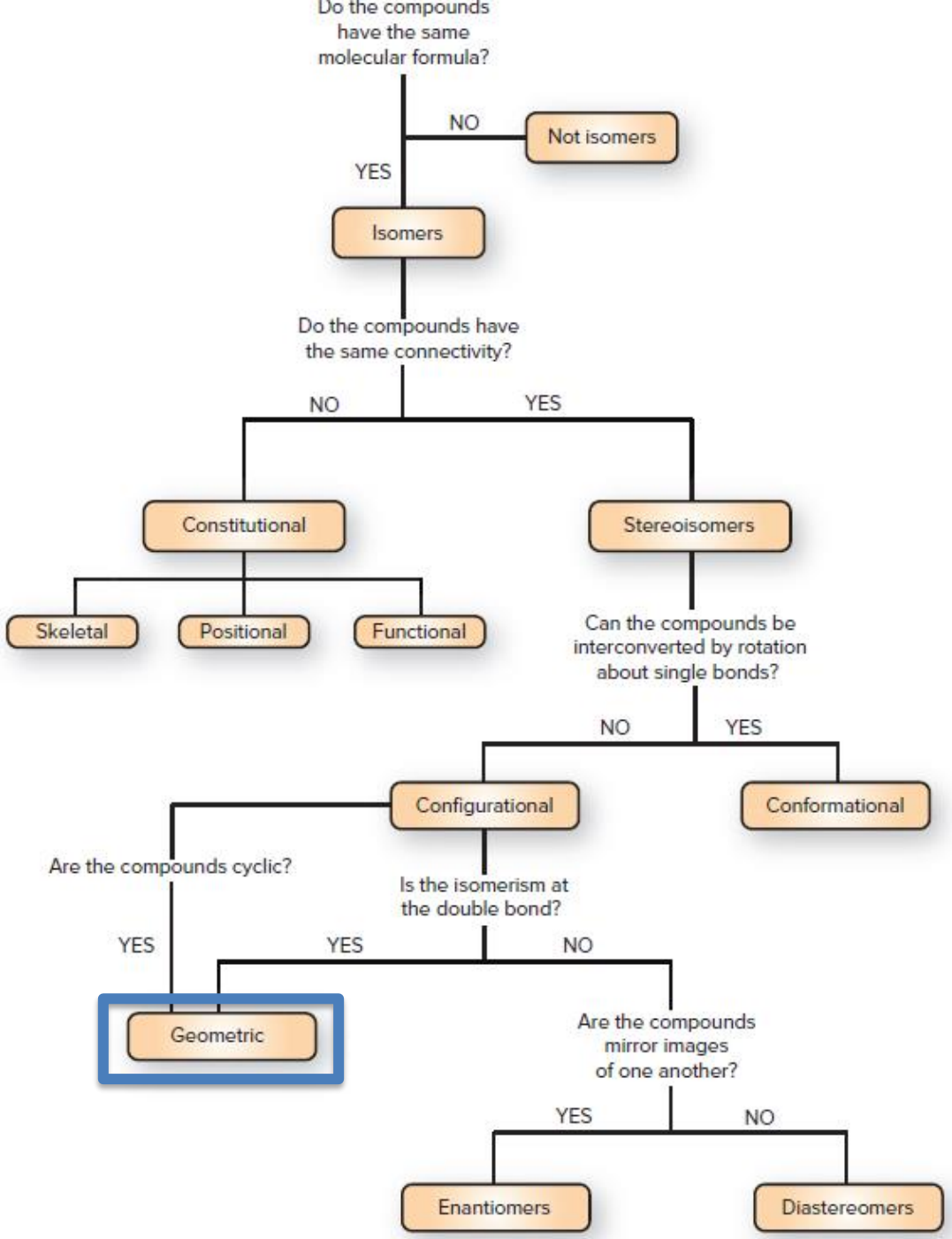
- unpaired electrons from p_z orbitals overlap side-to-side
- two electrons can move over new π -bonding molecular orbital
- no C-C bond rotation, would have to break π -bond





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

Isomers!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Is the isomerism at the double bond?
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Are the compounds mirror images of one another?
YES
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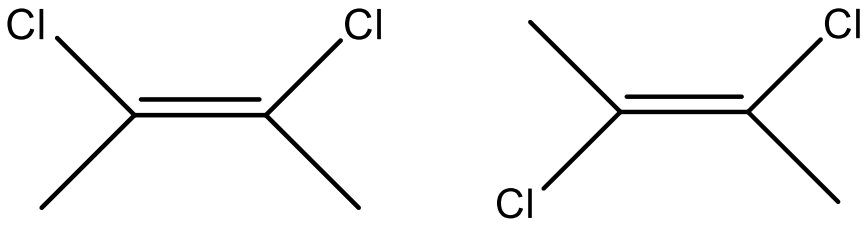
Enantiomers
Diastereomers

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

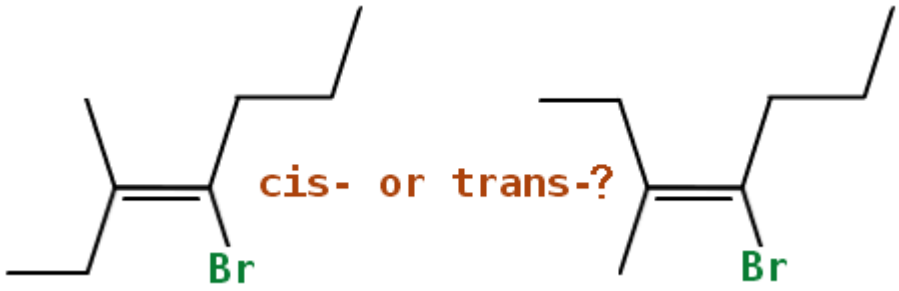
The more correct and common nomenclature is “E/Z”.
E = entgegen (opposite)
Z = zusammen (together)
E/Z based on “priority” not based on carbon chain length!
-priority = “heaviest” i.e. highest atomic number

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

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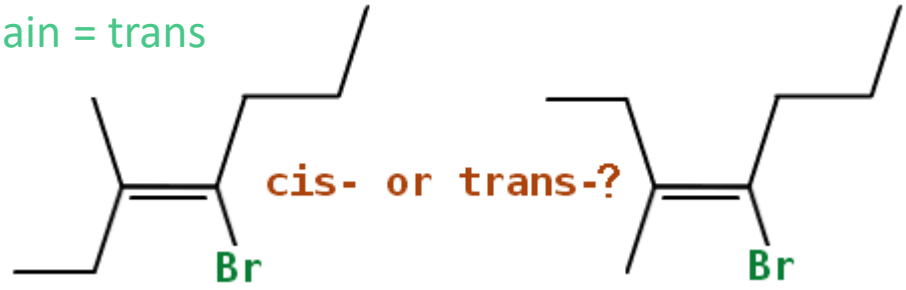
Z = zusammen (together)
E/Z based on “priority” not based on chain length!

Longest chain = 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!!!

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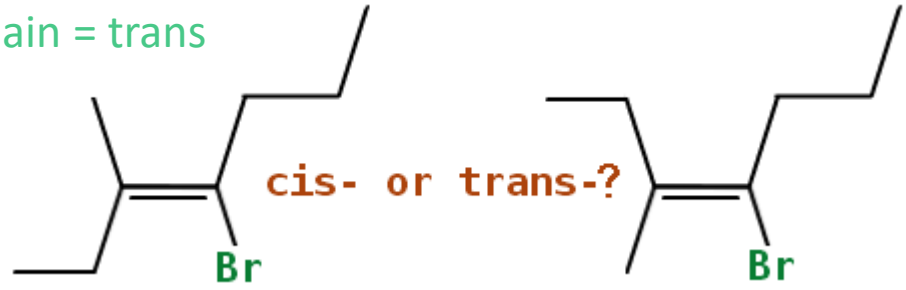
Longest chain = trans



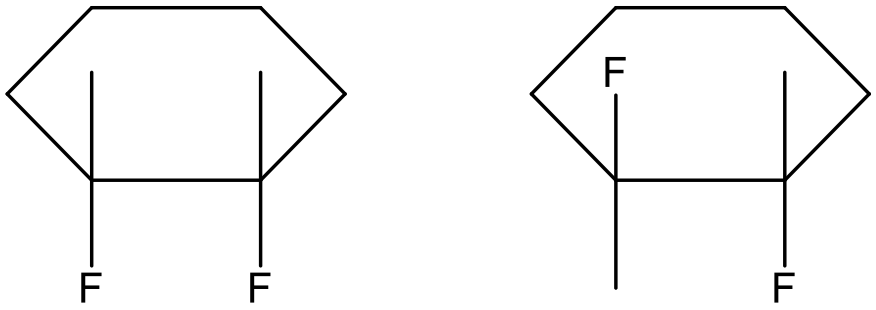
Longest chain = cis

Highest priority is opposite (E)

Highest priority is on the same side (Z)

Geometric Isomers (more examples)

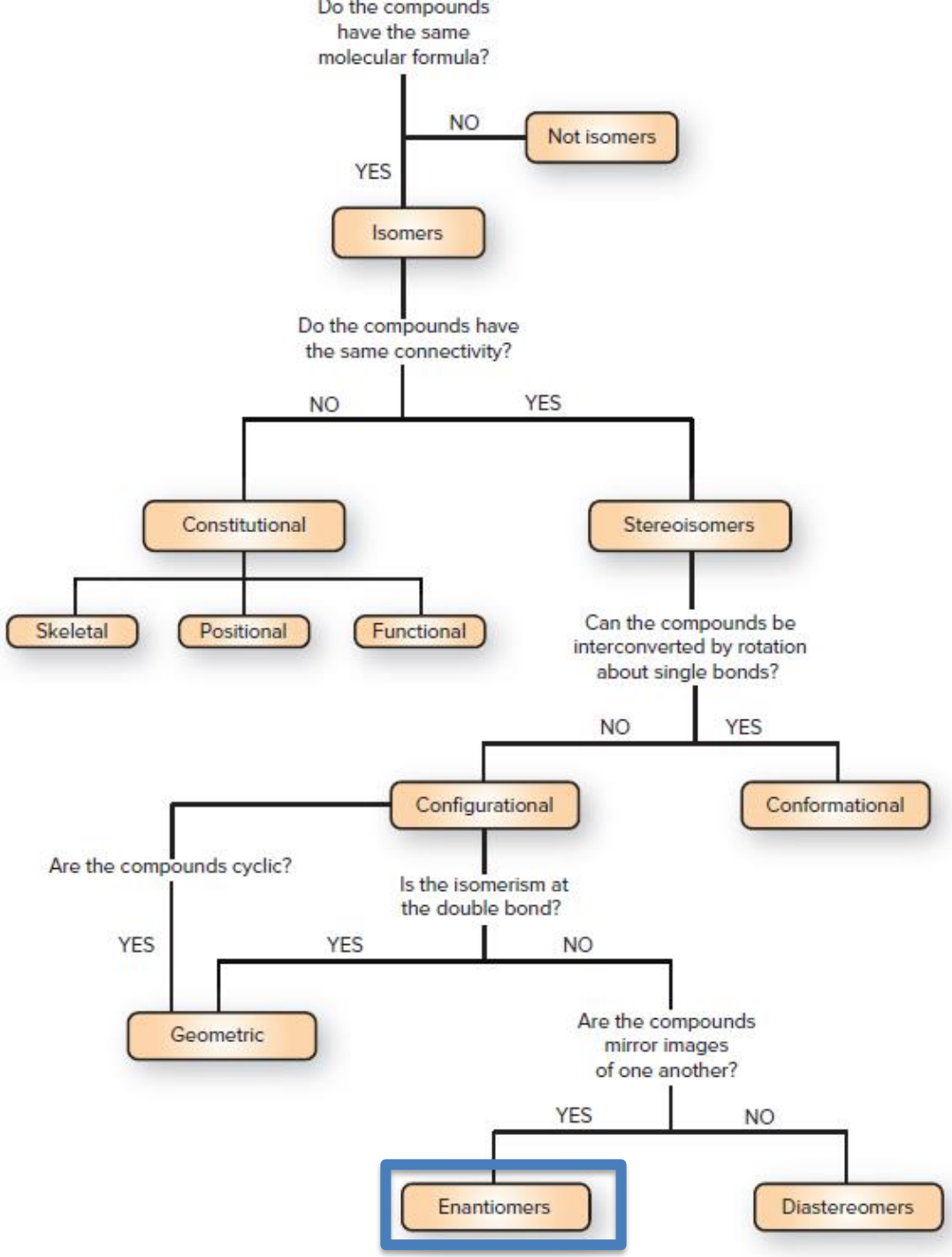
Same chemical formula same bonding different orientation of atoms – STEREOISOMERS



cis trans

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

Isomers!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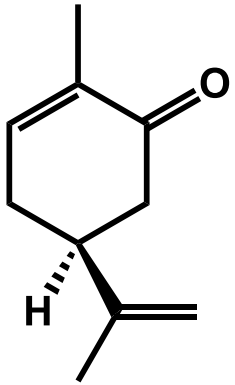
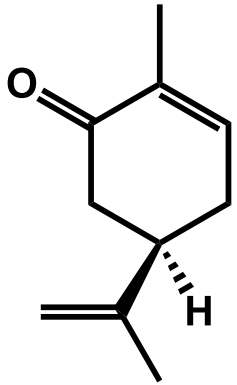
Configurational
Conformational
Are the compounds cyclic?
Is the isomerism at the double bond?
YES
YES
NO
Geometric
Are the compounds mirror images of one another?
YES
NO
Enantiomers
Diastereomers

STEREOISOMERS **2.Enantiomers**



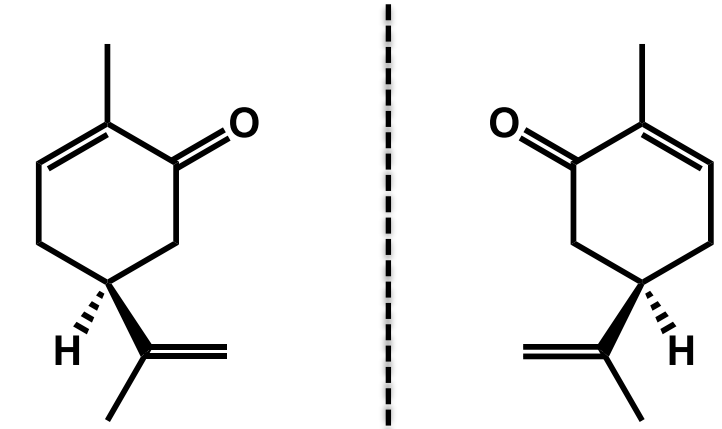
caraway



mint

Same chemical formula same bonding nonsuperimposable mirror images – Enantiomers

ENANTIOMERS AND CHIRALITY

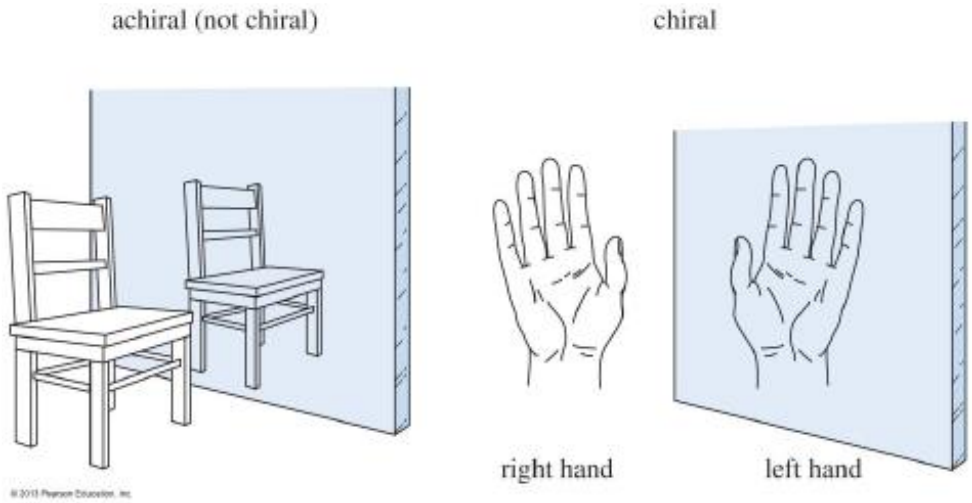


caraway mint

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

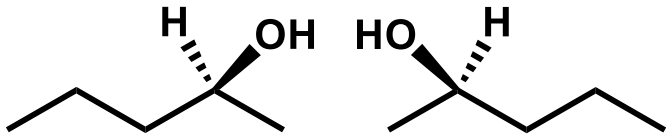
1. No plane of symmetry (can't cut it in half, or thirds etc, and get the same on one side as the other side!)

2. Must have a chiral center- 4 different groups (sp^3 hybridized)

2-propanol

ACHIRAL

SUPERIMPOSABLE MIRROR IMAGES

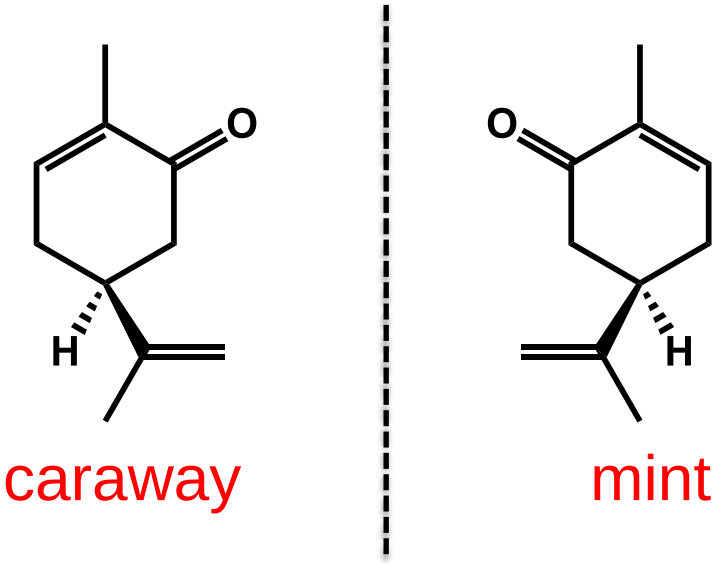


2-pentanol

CHIRAL

NON-SUPERIMPOSABLE MIRROR IMAGES

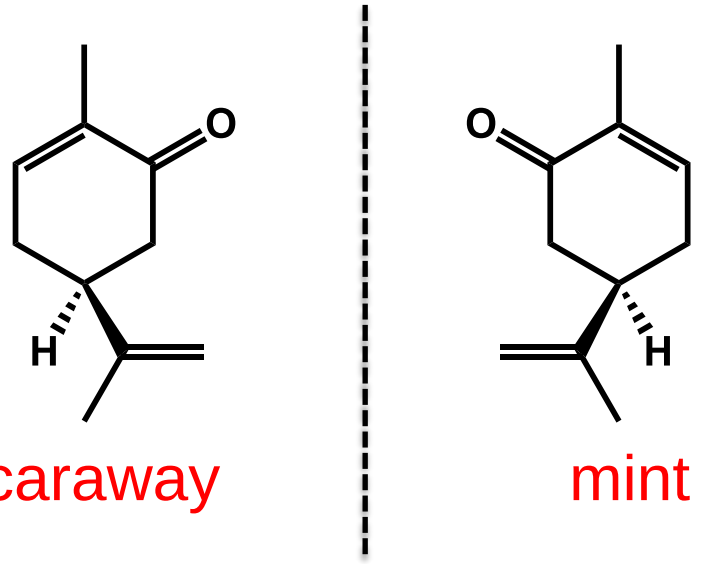
CHIRALITY AND ENANTIOMERS



caraway mint

Why do we care?

CHIRALITY AND ENANTIOMERS

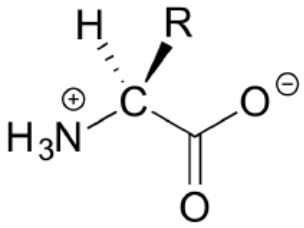


caraway mint

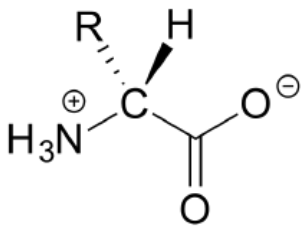
Enantiomers also show **similar chemical properties** **until** they react with another chiral compound!

Chiral molecules in the human body

Amino acids are chiral!

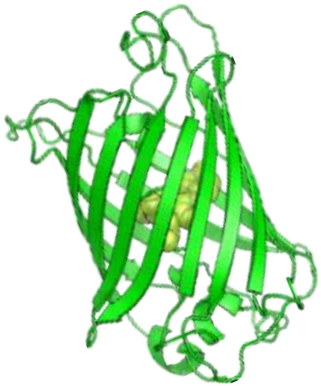


L-amino acids
(common in nature)

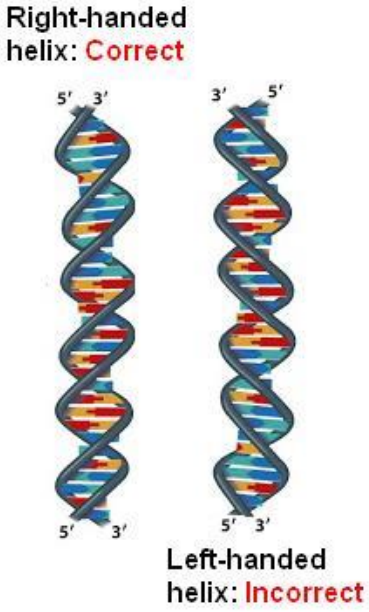


D-amino acids
(rare in nature)

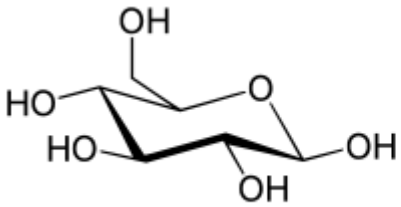
Proteins are chiral!



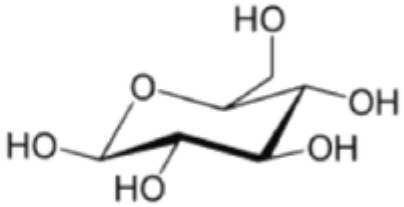
DNA is chiral



Carbohydrates (sugars) are chiral!



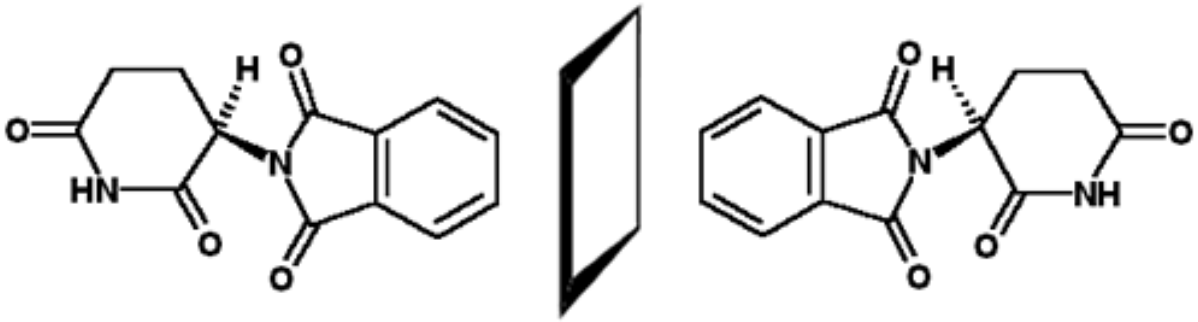
D-Glucose



L-Glucose

Found in nature

Drugs have to (sometimes) be *enantiopure*



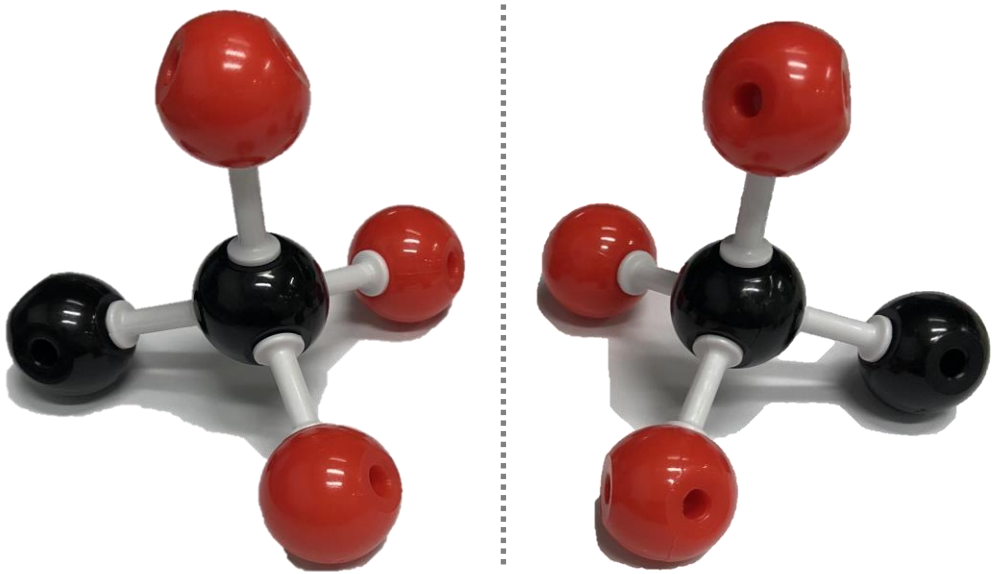
R-Thalidomide
(sleep-inducing)

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)**



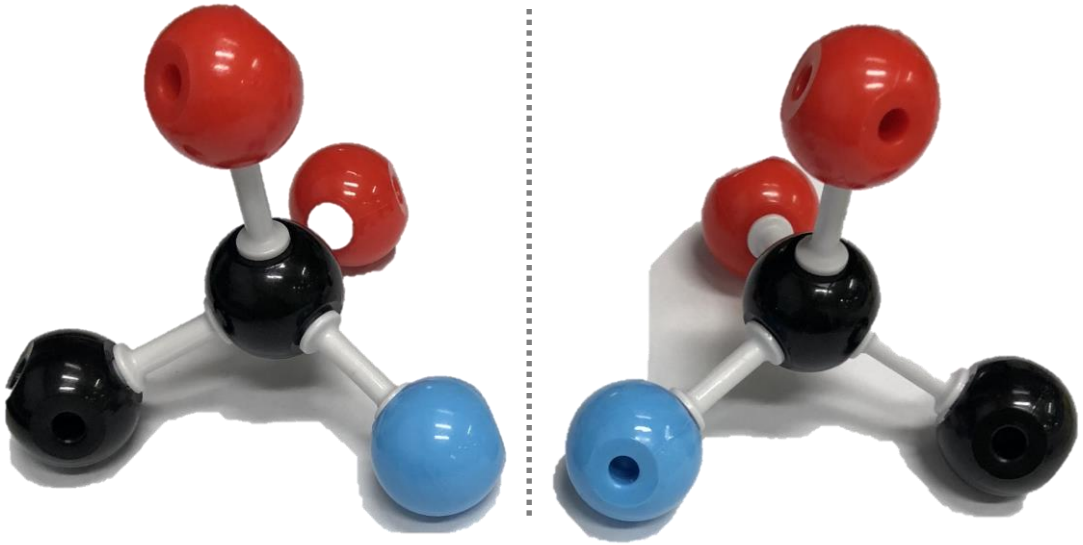
If you flip it, they will line up and look the same!

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)**



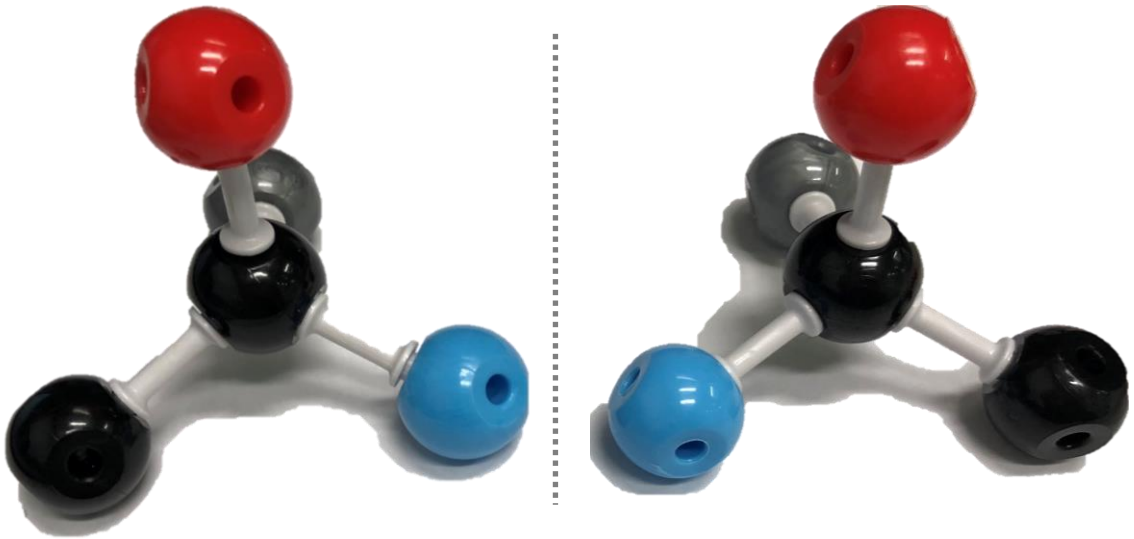
If you flip it, they will line up and look the same!

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)**

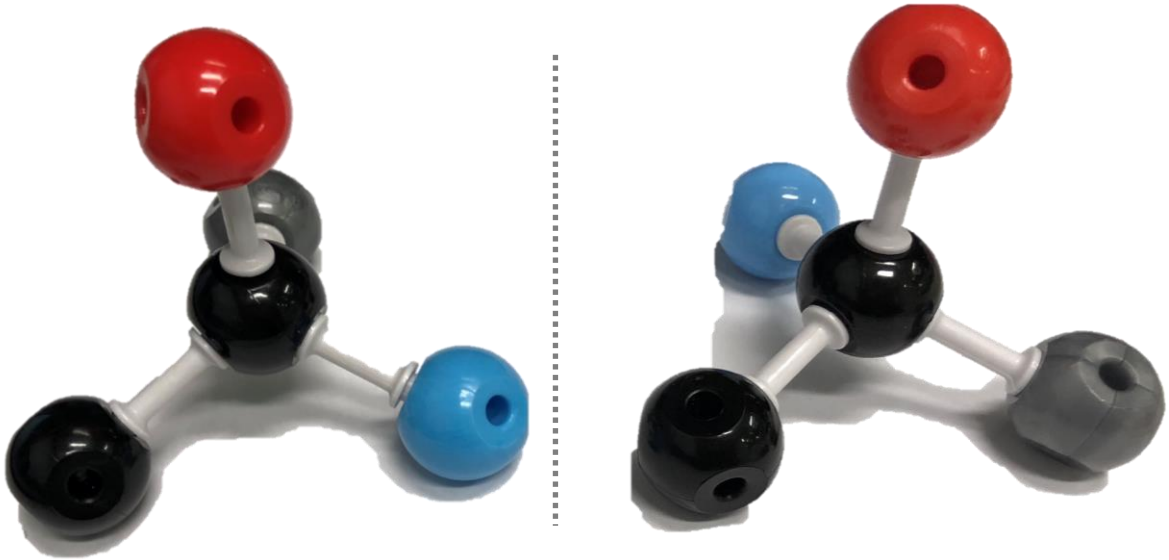


All four different substituents – these are nonsuperimposable mirror images – **these are enantiomers**

Are these enantiomers?

CHIRAL MOLECULE

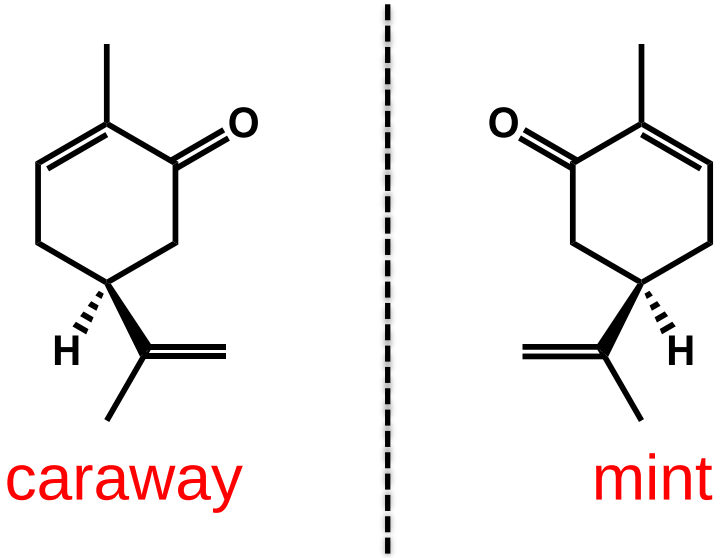
1. **No plane of symmetry**
2. **Must have a chiral center- 4 different groups (sp^3 hybridized)**



If you flip it, they do not ever match ☺

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

CHIRALITY AND ENANTIOMERS

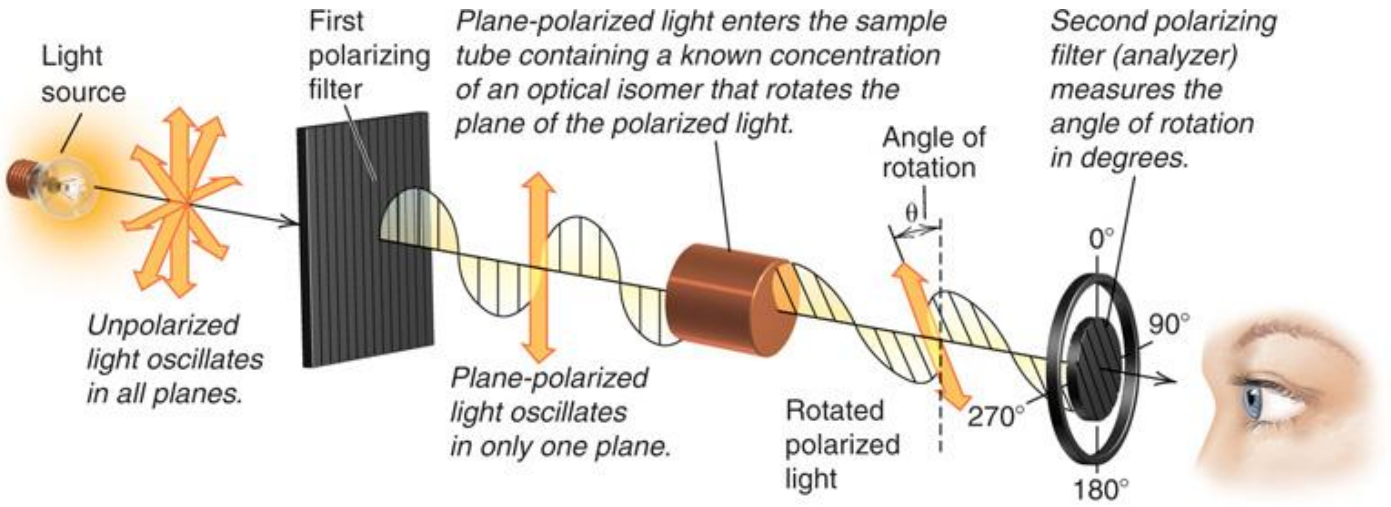


caraway mint

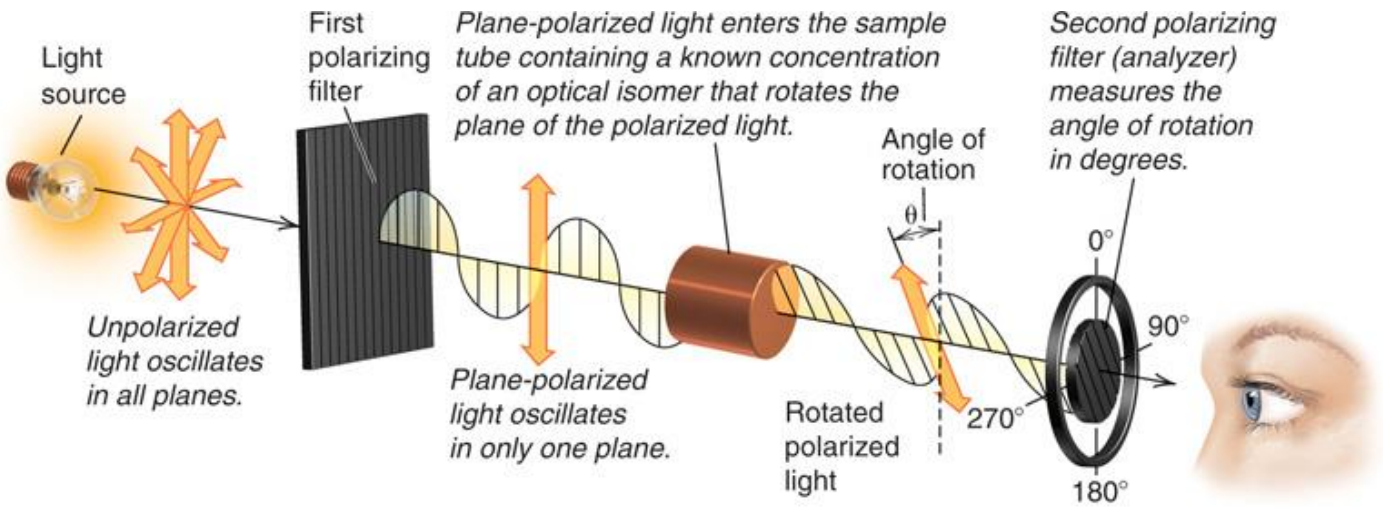
Enantiomers differ in one physical property: chiral molecules are optical activity, they can rotate plane polarized light. If a chiral molecule rotates light clockwise, then its mirror image rotates it counterclockwise.

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



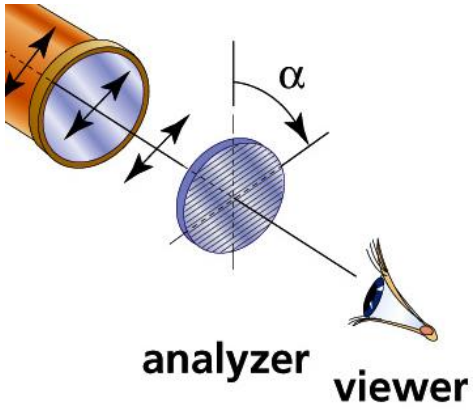
PHYSICAL PROPERTIES OF ENANTIOMERS

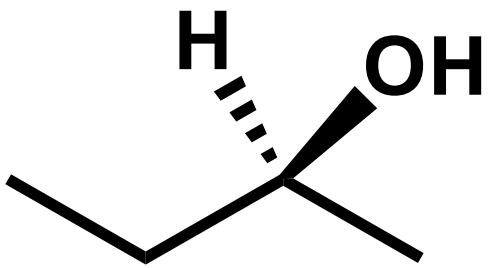


Based on optical rotation data: Enantiomers can be classified as dextrorotatory or levorotatory

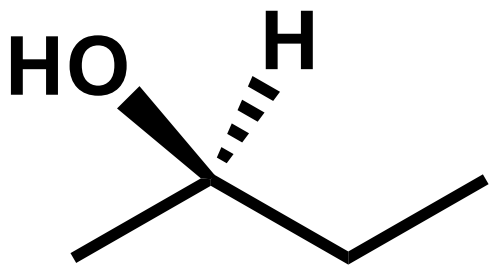
Enantiomers are OPTICALLY ACTIVE

RACEMIC MIXTURES





(+)-2-butanol



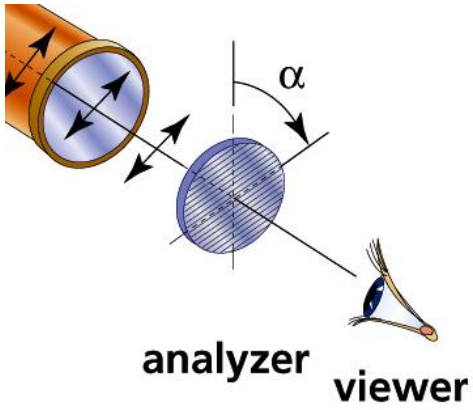
(-)-2-butanol

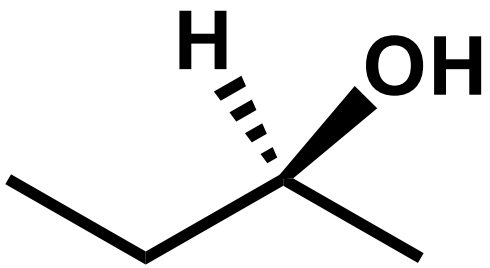
Specific rotation data

Clockwise rotation
+

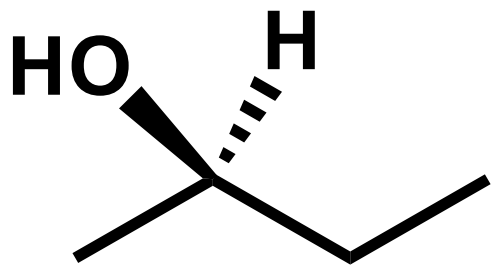
Counterclockwise rotation
-

RACEMIC MIXTURES





(+)-2-butanol



(-)-2-butanol

1 : 1 mixture of enantiomers

Racemic Mixture: Optically inactive

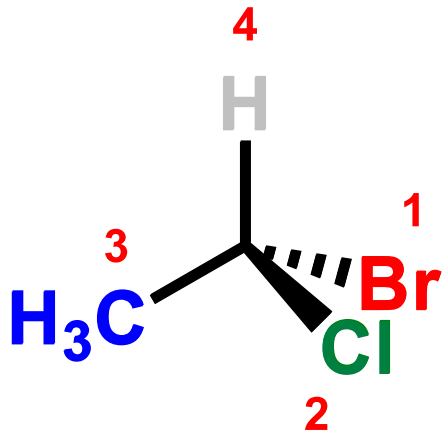
Naming Enantiomers: “R” or “S”

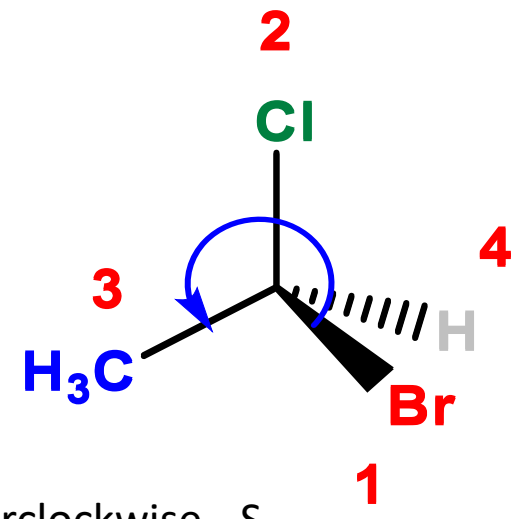
Only for Chiral centres:

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

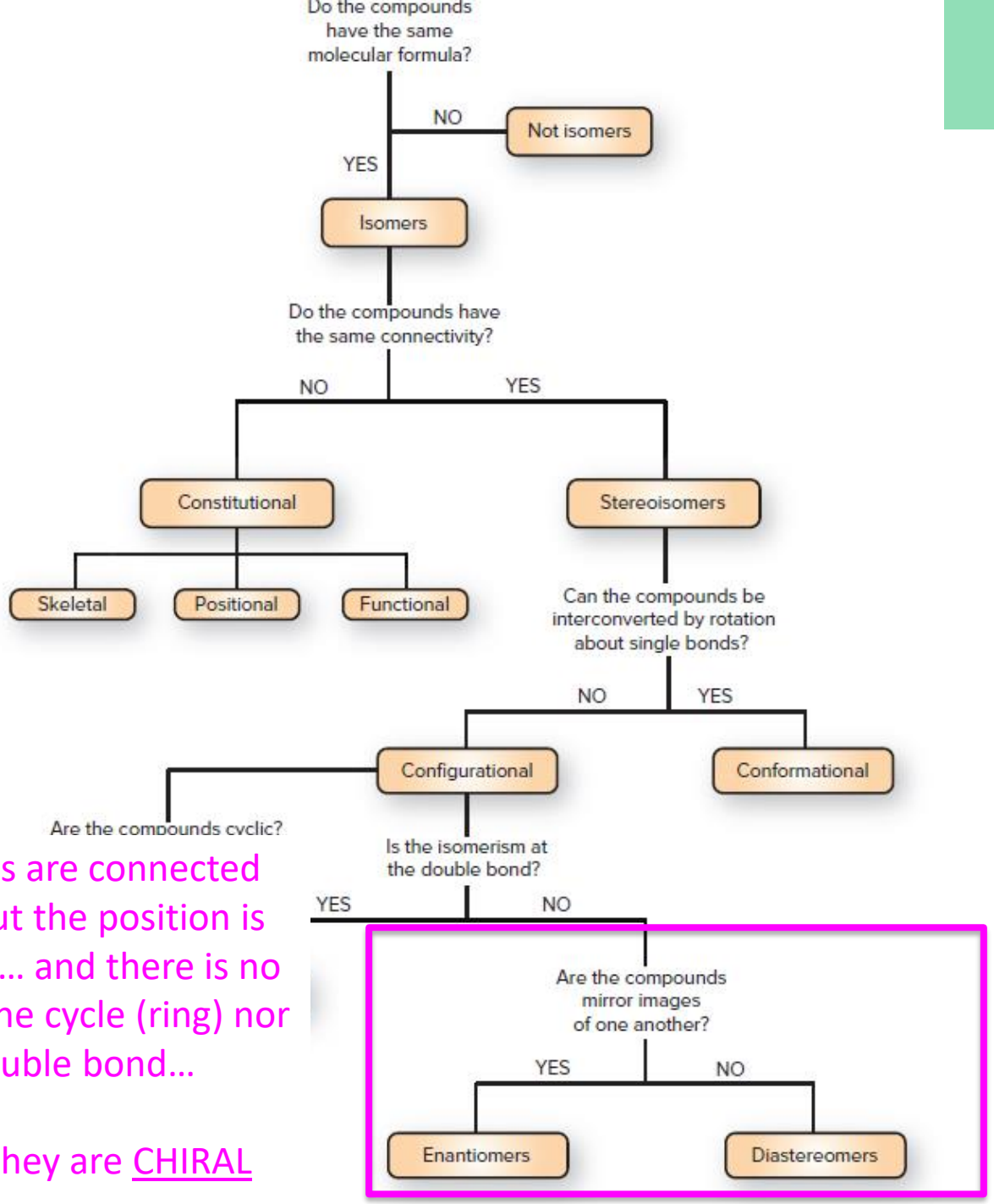
“S”: If the curved arrow is drawn counter-clockwise





Counterclockwise - S

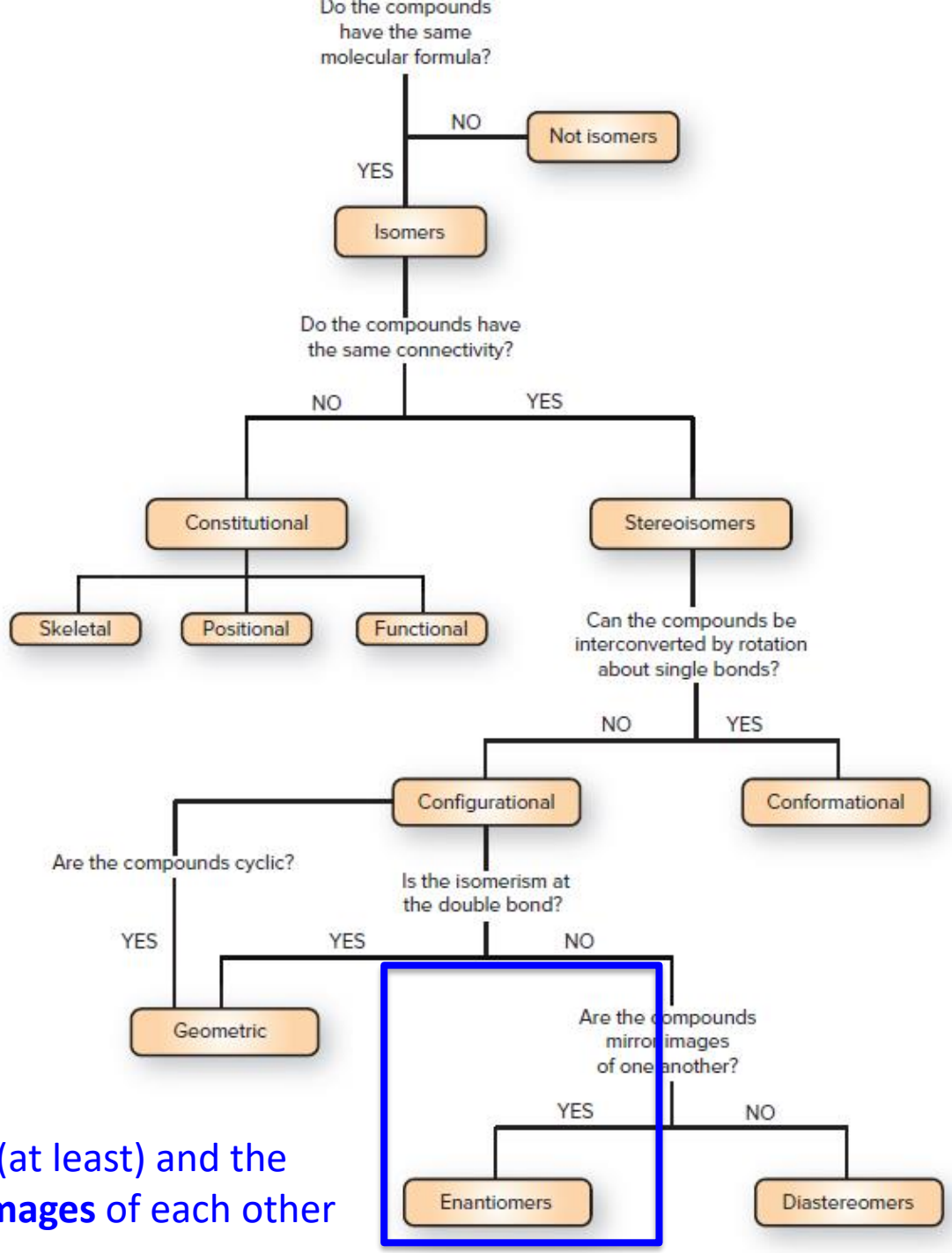
Isomers!



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…

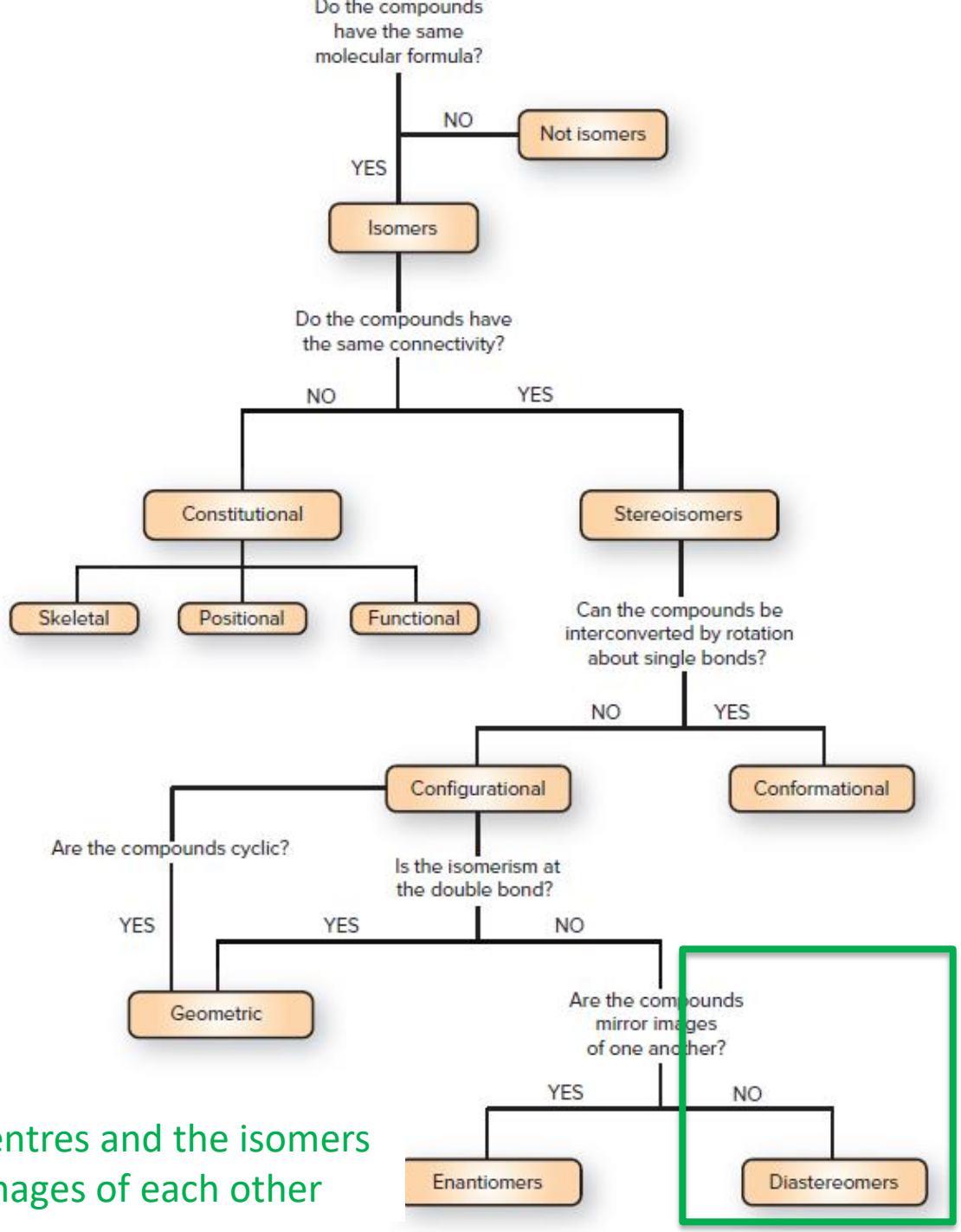
MUST be because they are CHIRAL

Isomers!



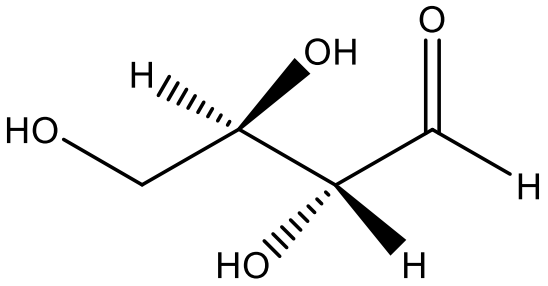
One chiral centre (at least) and the isomers are **mirror images** of each other

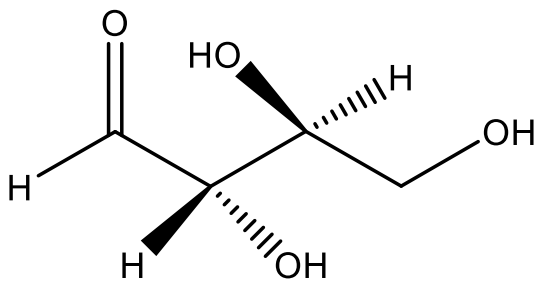
Isomers!



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

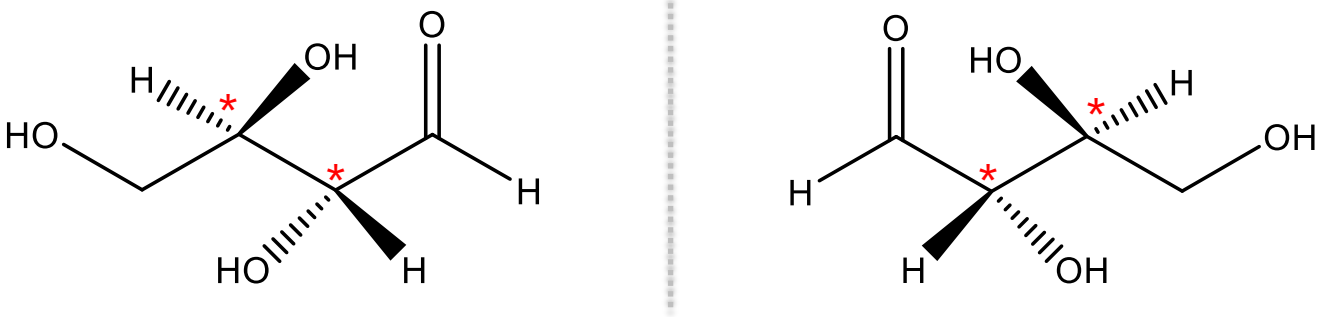
STEREOISOMERS 3: Diastereomers





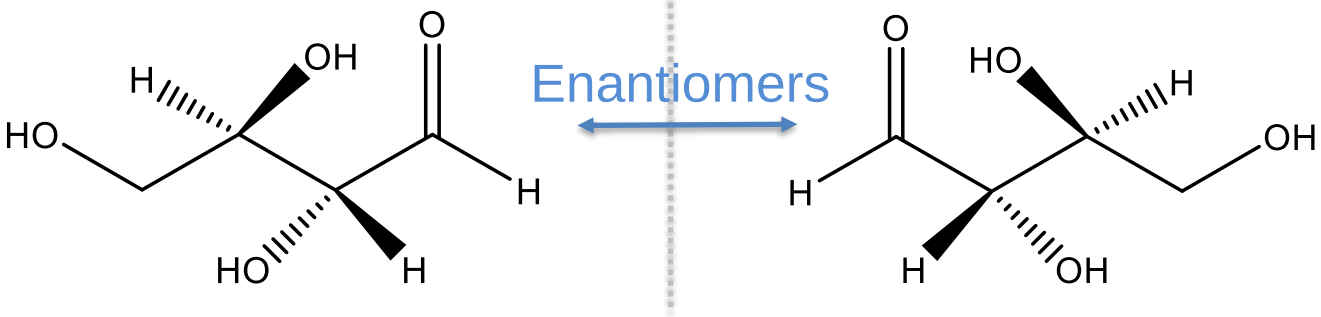
How many chiral carbons does this compound have?

STEREOISOMERS 3: Diastereomers

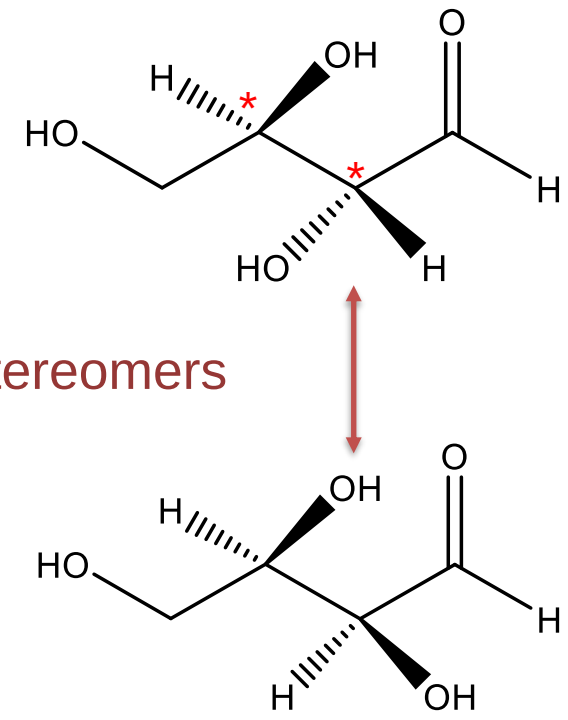


How many chiral carbons does this compound have? 2

STEREOISOMERS 3: Diastereomers

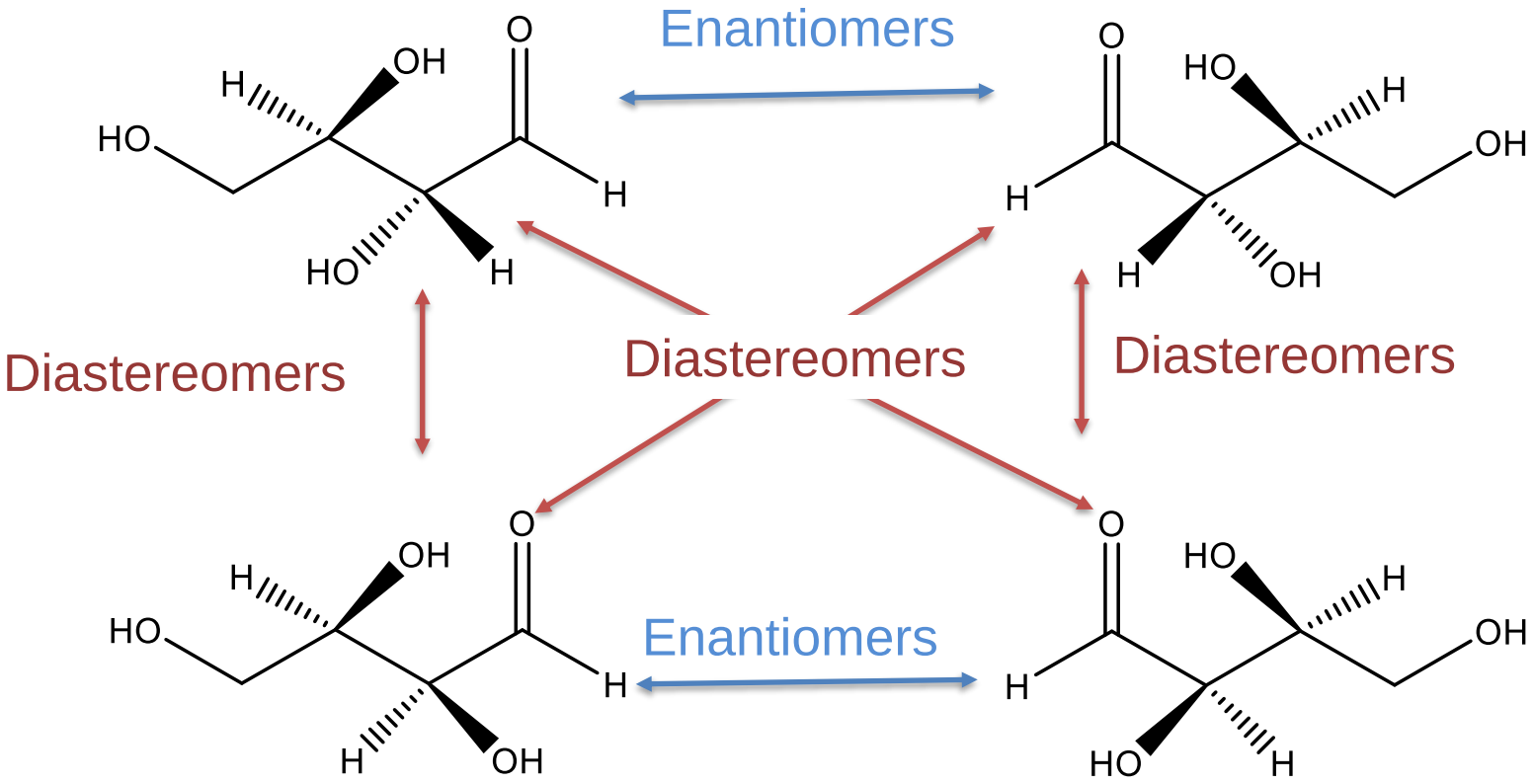


STEREOISOMERS 3: Diastereomers



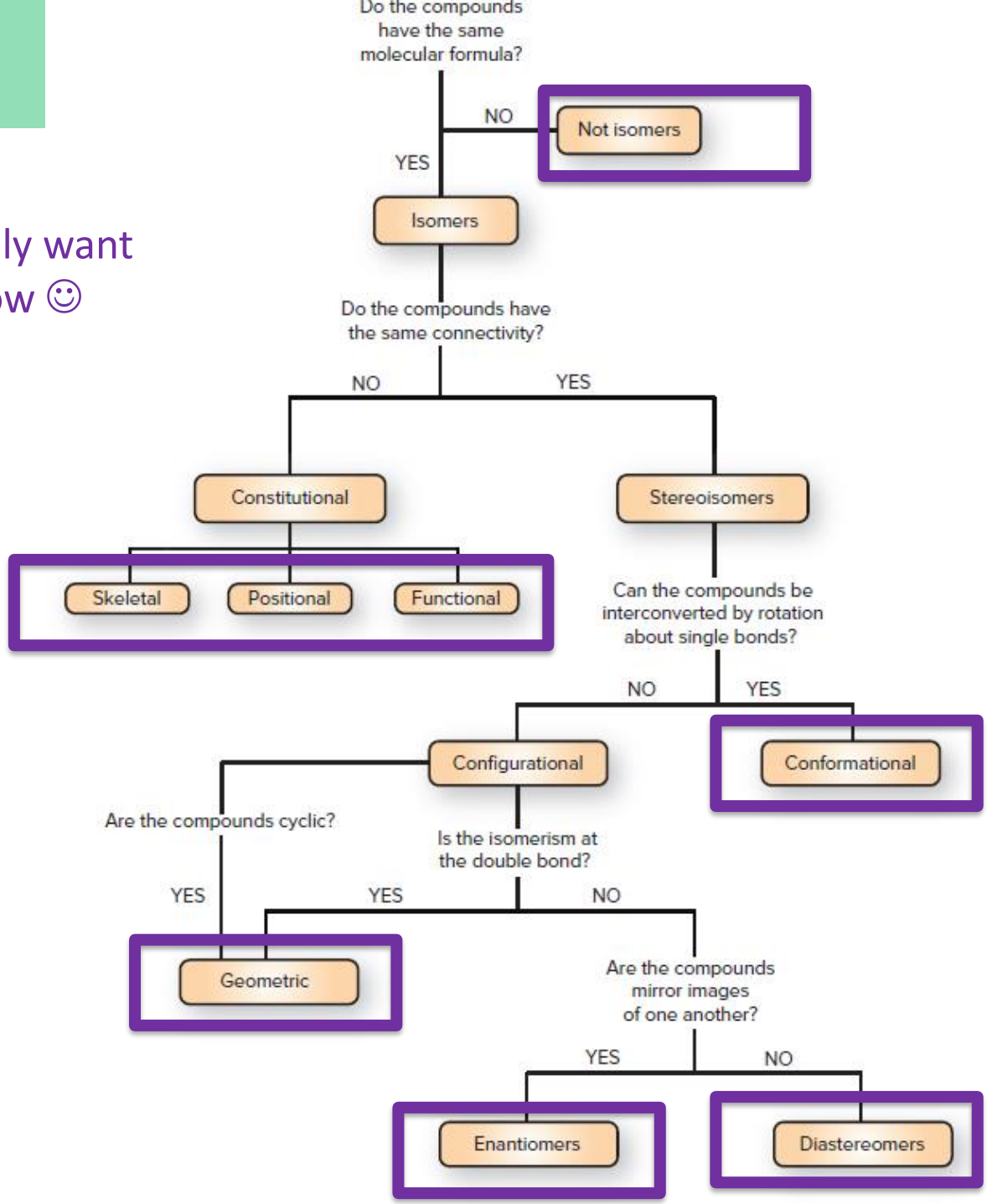
Same chemical formula same bonding non-mirror images stereoisomers - **Diastereomers**

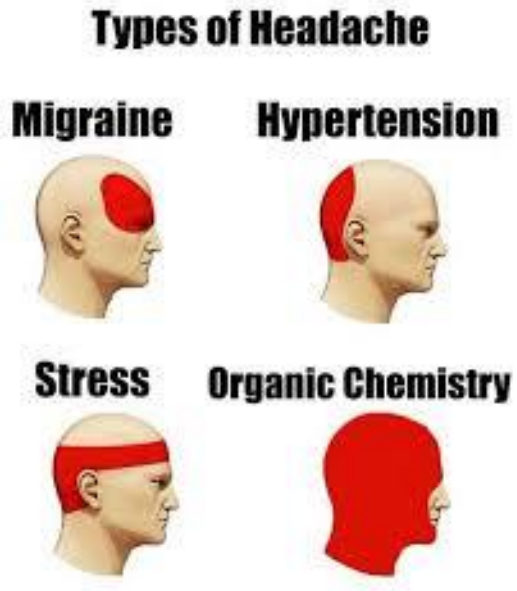
STEREOISOMERS 3: Diastereomers



Isomers!

What I actually want you to know ☺





Congrats you made it!