(22) **Today**

Sections 5.1 – 5.5
Chirality and Determining the Configuration of Chiral Centers

Sections 5.6 – 5.12
Diastereomers, N,P, and S, and Prochirality

Next Class (23)

Test 2 on Chap 2, Sections 2.7 through 2.12, Chap 3, and Chap 4.

(24) **Second Class from Today**

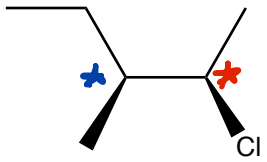
Sections 5.6 – 5.12
Diastereomers, N,P, and S, and Prochirality

Third Class from Today (25)

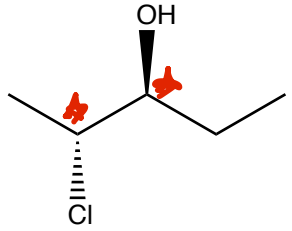
Section 6.1: Kinds of Organic Reactions
Section 6.8: Describing a Reaction: Bond Dissociation Energies
Section 6.7: Describing a Reaction: Equilibria, Rates, and Energy Changes
Section 6.2: How Organic Reactions Occur: Mechanisms
Section 6.9: Describing a Reaction: Energy Diagrams and Transition States
Section 6.10: Describing a Reaction: Intermediates

Review session, Tuesday 7:30 - 9:00 pm
watch email for a room announcement.

H
CH_3
CH_2CH_3
stuff

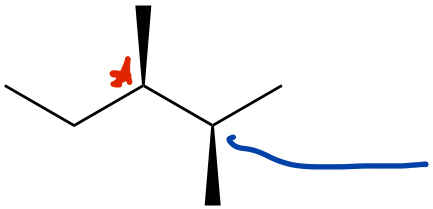


H
CH_3
Cl
stuff



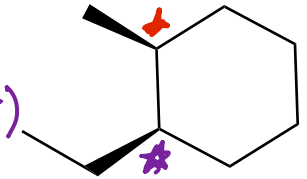
CH_3, H, CH_2, CH(C)

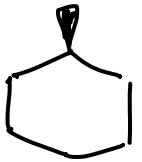
CH_3, H, Et, i-Pr



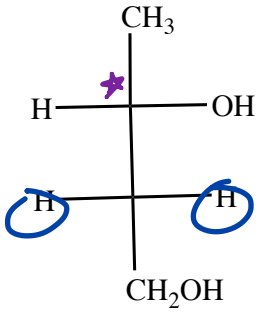
H
CH_3
CH_3
stuff

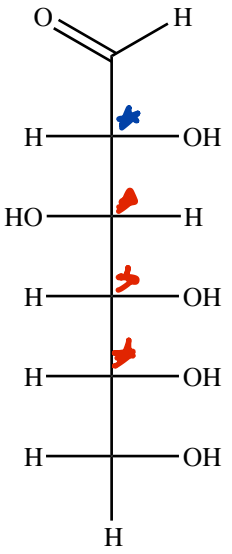
H, Et,
CH_2, CH(C)





CH, H





Definitions

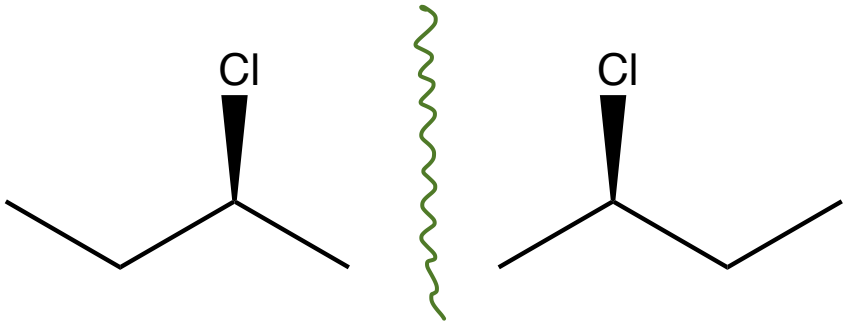
stereoisomers are molecules that have the same connectivity but different 3-D relationships between parts of the molecules

e.g. (*R*)-2-chlorobutane vs (*S*)-2-chlorobutane

The word **enantiomer** describes the relationship between two stereoisomers.

enantiomers are stereoisomers that are nonsuperposable mirror images of each other and an object must be chiral to have an enantiomer

e.g. (*S*)-2-chlorobutane vs (*R*)-2-chlorobutane



left right mirror

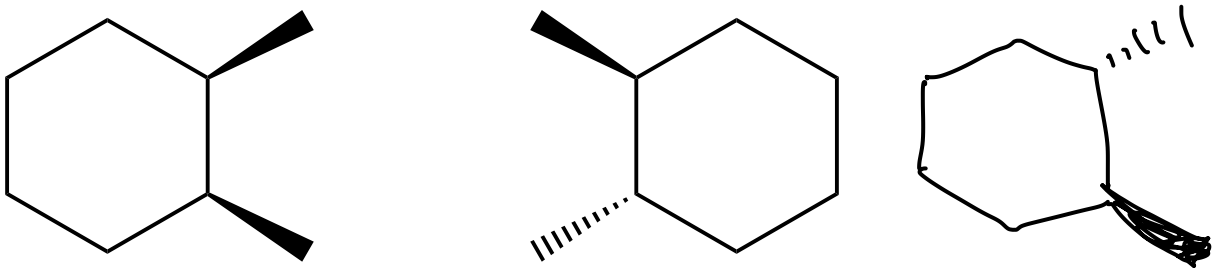
Definitions

stereoisomers are molecules that have the same connectivity but different 3-D relationships between parts of the molecules

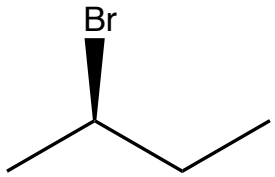
e.g. (*cis*)-1,2-dimethylcyclohexane vs (*trans*)-1,2-dimethylcyclohexane

The word **diastereomer** describes the relationship between two stereoisomers.

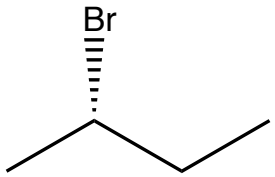
Diastereomers are stereoisomers that are nonsuperposable but are **NOT** mirror images of each other



Recognizing Enantiomers and Diastereomers: Why is it important?



BP = 91 °C



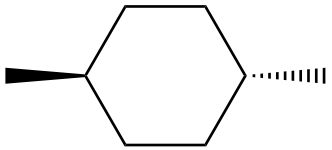
BP = 91 °C*

enantiomers have the same physical properties

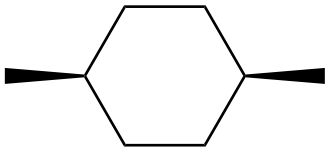
same chemical properties

Interact with chiral objects differently

Interact with polarized light differently



BP = 119 °C†

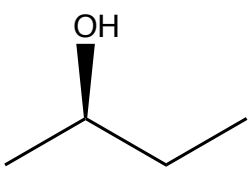


BP = 125 °C††

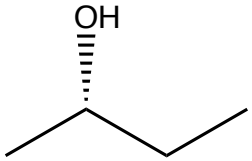
Different chemical & physical properties

*https://en.wikipedia.org/wiki/2-Bromobutane
†https://us.vwr.com/store/product/16811100/trans-1-4-dimethylcyclohexane-95-0-by-gc
††https://us.vwr.com/store/product/9559540/cis-1-4-dimethylcyclohexane-98-0

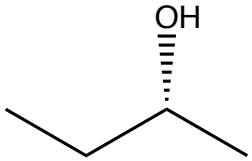
Front-back

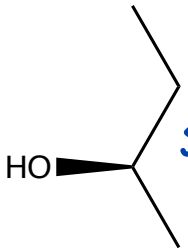


A



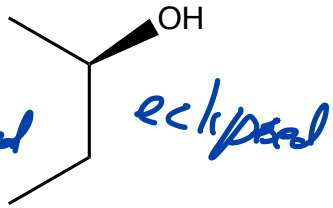
B





C

staggered



D

eclipsed

different view of the same molecule/rotamer or enantiomer or diastereomer

A is an enantiomer

B is a dif view

C is a dif view

D is a dif view of a rotamer

rotate along a bond

nonsuperposable mirror image

nonsuperposable not mirror image

Assign Priorities

highest priority is given to the group with the highest atomic number for the atom directly bonded to the chirality center

in a tie, consider the atomic numbers of the atoms attached to the atom that is bonded to the chirality center

if the atom that is attached to the chirality center has a doubly bonded or triply bonded atom attached to it the atom is treated like there are two or three atoms

for isotopes, the mass number is used (D vs H, ^{12}C vs ^{13}C)

Point lowest priority group away

Draw a circle from 1st to 2nd to 3rd priority groups

Clockwise circle is **R** configuration

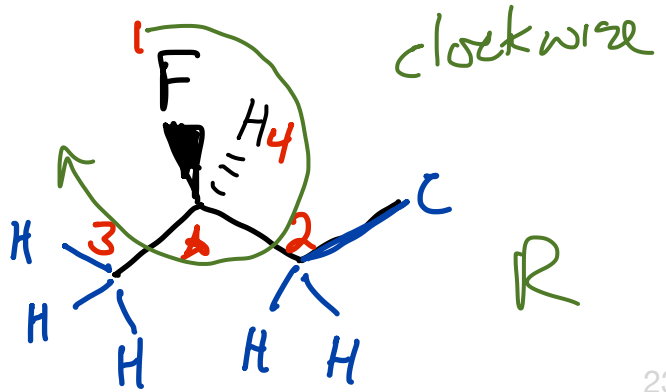
Counter Clockwise circle is **S** configuration

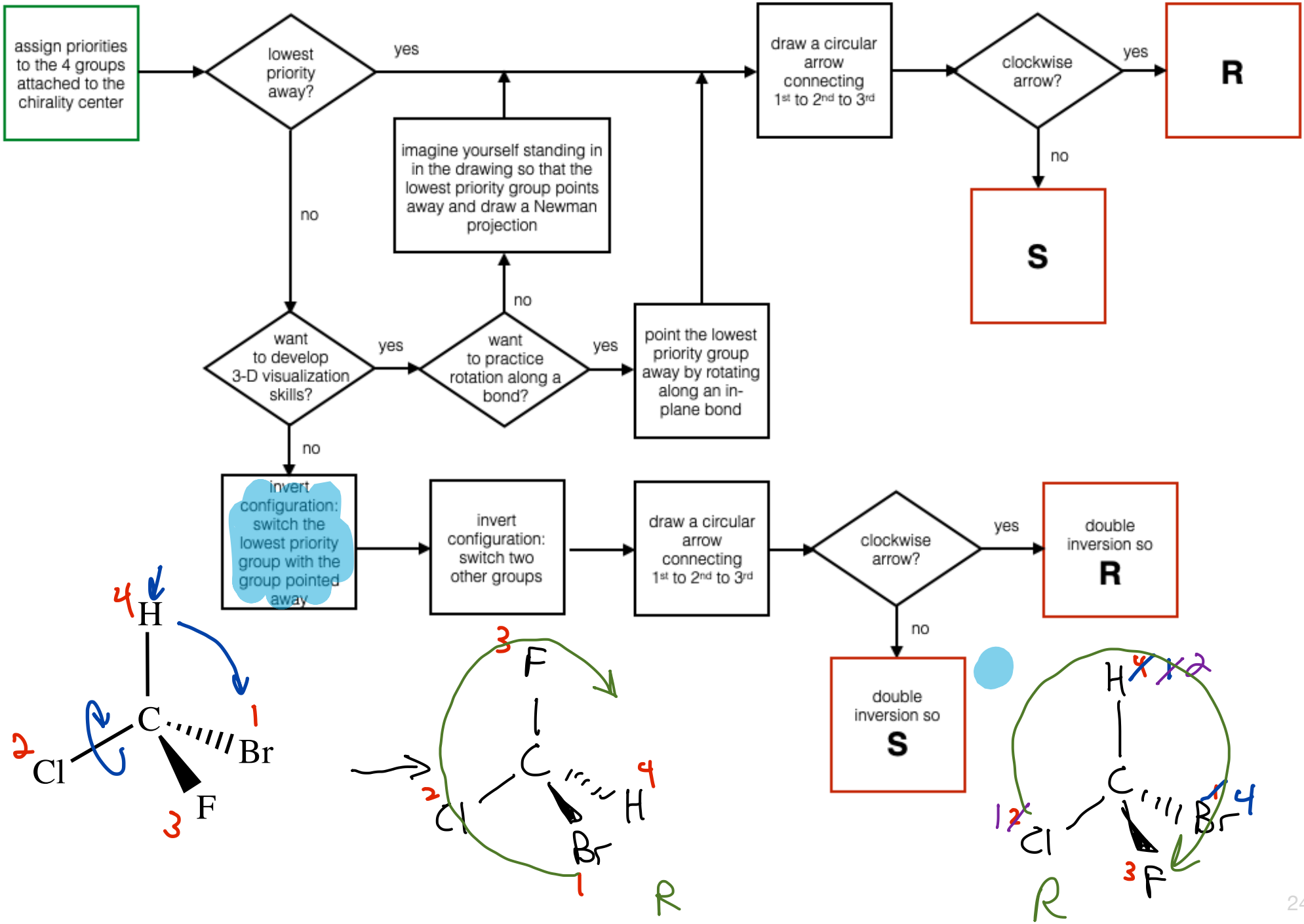
Z = 9 F 1st

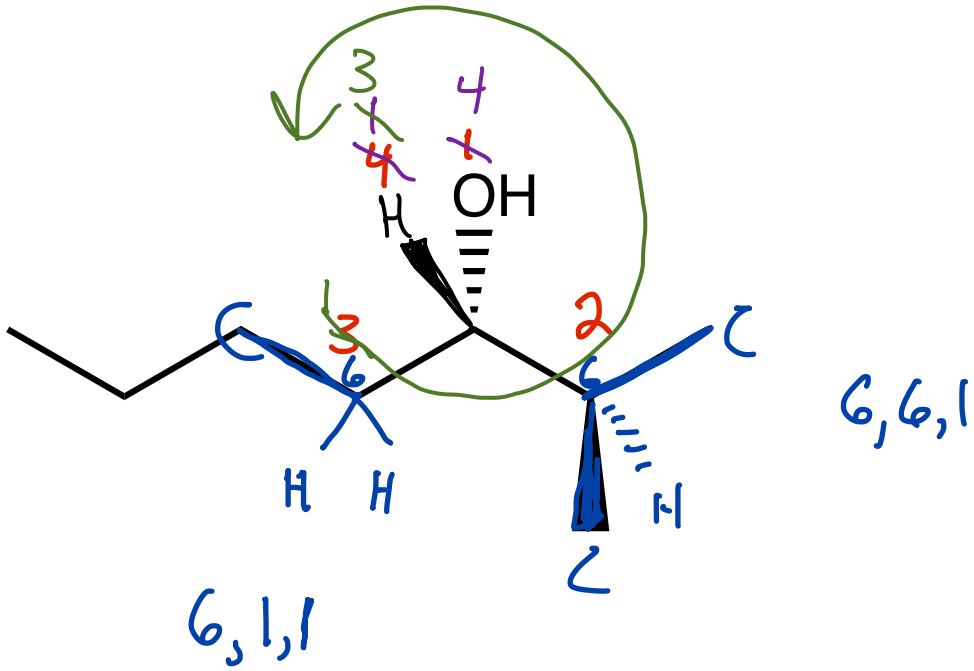
Z = 1,1,1 Z = 6 CH_3 3rd

Z = 1,1,6 Z = 6 CH_2CH_3 2nd

Z = 1 H 4th



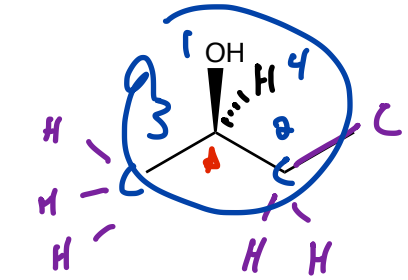

assign priorities to the 4 groups attached to the chirality center
lowest priority away?
yes
no
draw a circular arrow connecting 1st to 2nd to 3rd
clockwise arrow?
yes
R
no
S
imagine yourself standing in in the drawing so that the lowest priority group points away and draw a Newman projection
want to develop 3-D visualization skills?
yes
want to practice rotation along a bond?
yes
no
point the lowest priority group away by rotating along an in-plane bond
no
invert configuration: switch the lowest priority group with the group pointed away
invert configuration: switch two other groups
draw a circular arrow connecting 1st to 2nd to 3rd
clockwise arrow?
yes
double inversion so R
no
double inversion so S
H
Cl
Br
F
C
R
R


3
4
OH
H
2
C
C
C
H H
H
C
6,6,1
6,1,1
S

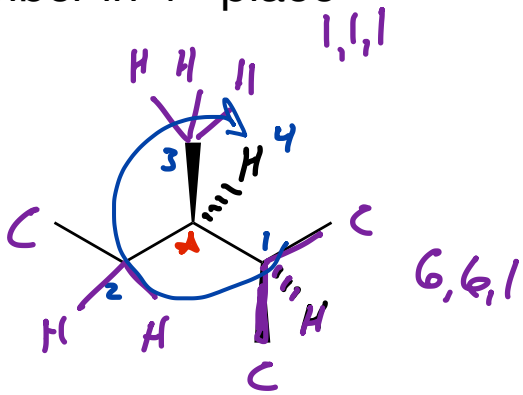
Priorities are based on the atomic number of the atoms bonded to the chiral center.

Highest atomic number is 1st place to lowest atomic number in 4th place

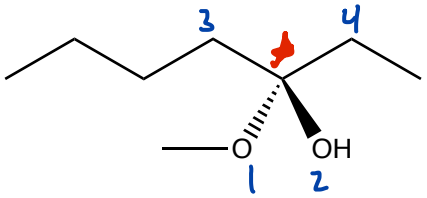
In a tie, go one bond further out.



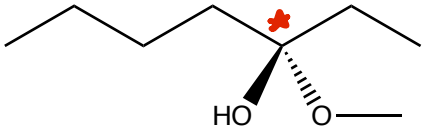
R



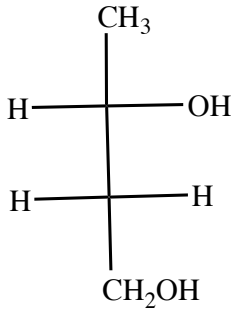
R

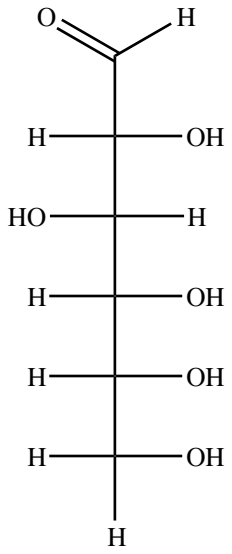


S

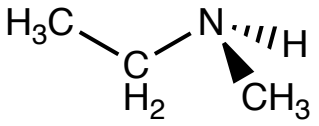


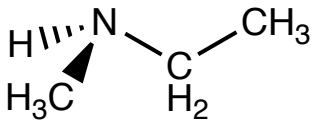
S

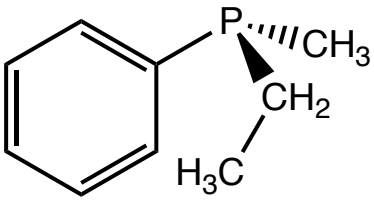

CH3
H
OH
H
H
CH2OH

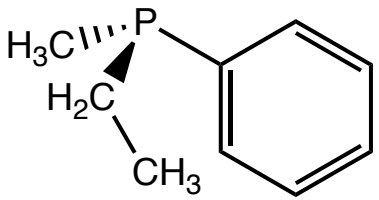

O
H
H
OH
HO
H
H
OH
H
OH
H
OH
H

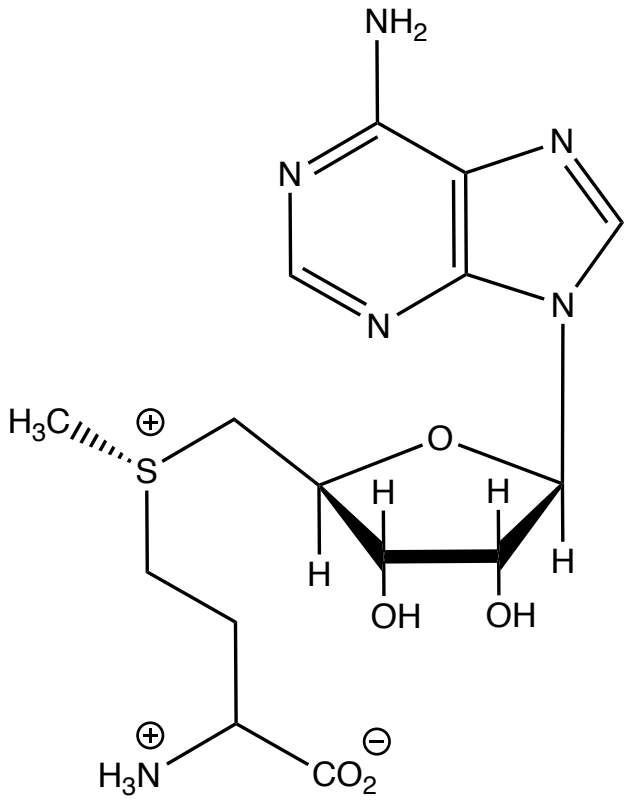
N and P Chirality Centers?





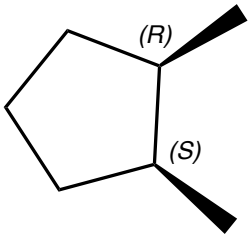


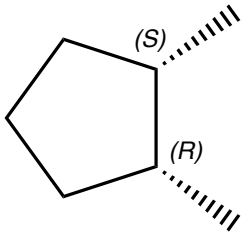


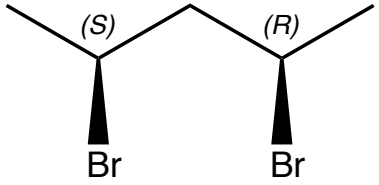


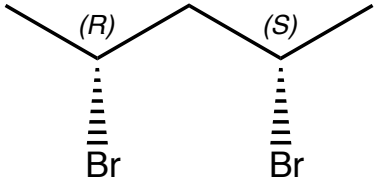
(*S*)-S-adenosylmethionine

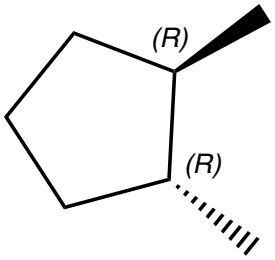
Enantiomers		Diastereomers
molecules that are **nonsuperposable** and **mirror images** of each other		molecules that have the same connectivity and are **nonsuperposable** but **NOT mirror images** of each other
The relationship can be identified using *R*,*S* system of nomenclature		
If all chirality centers in a chiral molecule have opposite configurations and Z,E alkenes, if present, remain the same There's a big BUT…		In molecules with more that one chirality center at least one pair but not all pairs of chirality centers have opposite configurations. In molecules with stereogenic alkenes (*Z*/*E* configuration) the alkenes have opposite configurations

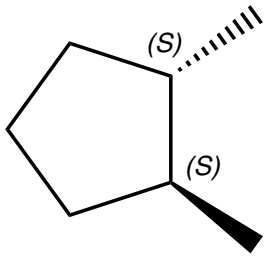

(R)
(S)

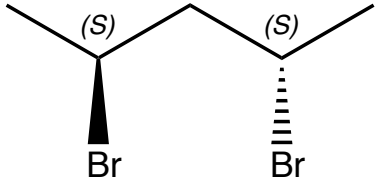

(S)
(R)

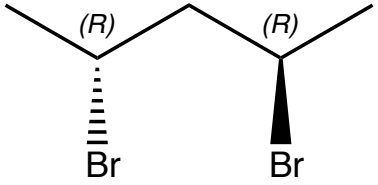

(S)
(R)
Br
Br


(R)
(S)
Br
Br


(R)
(R)

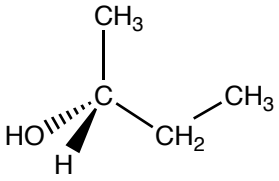

(S)
(S)

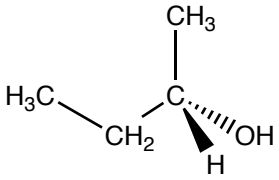

(S)
(S)
Br
Br

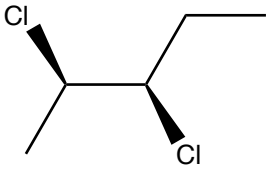

(R)
(R)
Br
Br

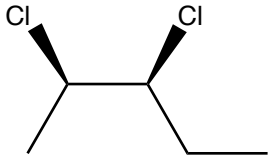
Enantiomers		Diastereomers
molecules that are **nonsuperposable** and **mirror images** of each other		molecules that are stereoisomers **nonsuperposable** but **NOT mirror images** of each other
The relationship can be identified using *R*,*S* system of nomenclature		
If all chirality centers in a chiral molecule have opposite configurations and Z,E alkenes, if present, remain the same Unless the compound is a meso complex Can occur when chirality centers have the same four different groups bonded to each chirality center		In molecules with more that one chirality center at least one pair but not all pairs of chirality centers have opposite configurations. In molecules with stereogenic alkenes (*Z*/*E* configuration) the alkenes have opposite configurations. In a chiral cyclic molecules with *cis*/*trans* relationships the *cis*/*trans* relationship changes

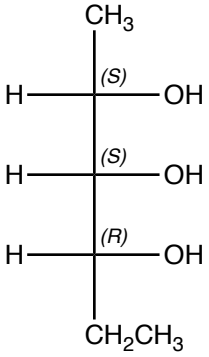
Practice Recognizing Relationships between molecules

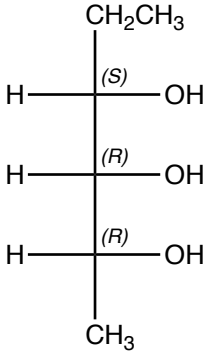


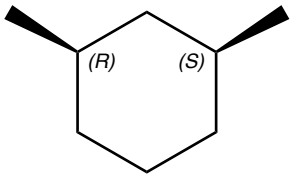


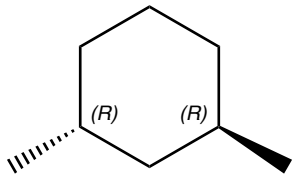


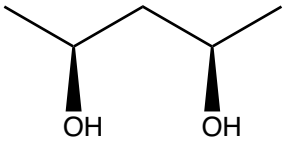


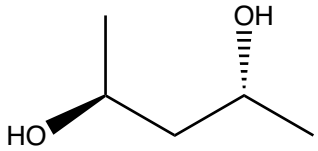


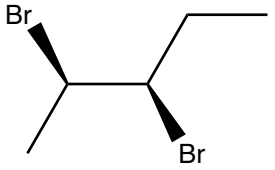


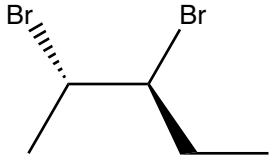












1. Draw a tetrahedral C atom

2. Assign priorities to the groups

3. Place the lowest priority group so that it points away

4. Draw in priority groups 1 through 3 in the correct (clockwise or counterclockwise) orientation.

(*R*)-2-chloropentane

(2*S*,3*S*)-2-bromo-3-chloropentane

1. Draw the molecule

2. Assign priorities and check if the correct configuration is drawn

3. a. If correct, celebrate, you're done

3. b. If incorrect version is drawn, redraw molecule switching the positions of 2 (and only two) substituents.

(*R*)-2-chloropentane

(2*S,3*S)-2-bromo-3-chloropentane