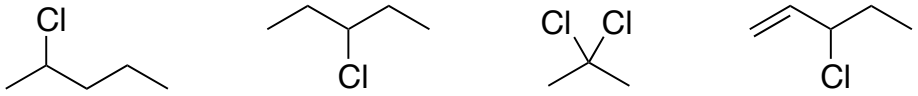
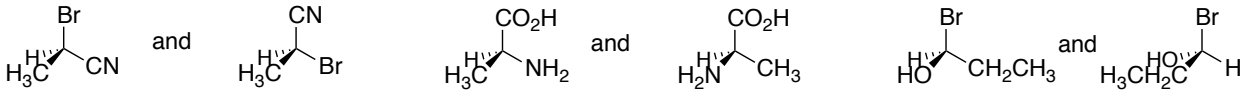
CHAPTER 5: STEREOCHEMISTRY

Identifying Chiral Carbons and Chirality.

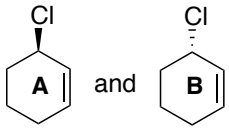
Which molecules contain chiral carbons? Mark the chiral carbons with an asterisk.



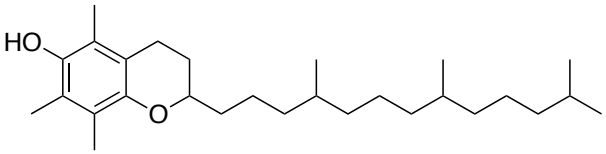
Without determining stereochemical configuration (R or S), can you determine which of the following pairs of molecules are the same, and which are enantiomers?



For molecules that have only one chiral atom, there can only be two possible isomers (below, left). If you count the number of chiral atoms and solve for 2^n, where n = # chiral atoms, this will tell you how many stereoisomers are possible for any given molecule. For example, $2^1 = 2$.



only two possible stereoisomers are possible for 3-chlorocyclohexene



1. Identify the chiral carbons
2. How many possible stereoisomers are can you have for this molecule?

Is molecule **A** optically active? _____

Is molecule **B** optically active? _____

Can you predict the optical rotation of **A** or **B**? _____

If you were to consider an equal mixture (1:1) of both **A** and **B**, could you predict the optical rotation of the mixture? _____

What is the name for this kind of mixture? _____

Naming Chiral Centers - The *R,S* System. Since we cannot assign D (or +) or L (or -) to an enantiomer simply based on its structure, another naming system must be used to distinguish between stereoisomers. After all, we can't name both these molecules 2-chloropentane.

2-chloropentane?

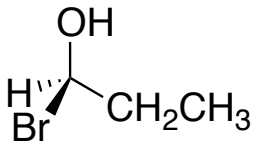
The Cahn-Ingold-Prelog priority rules are in place to specify an *absolute configuration* around a chiral center (carbon, in these examples).

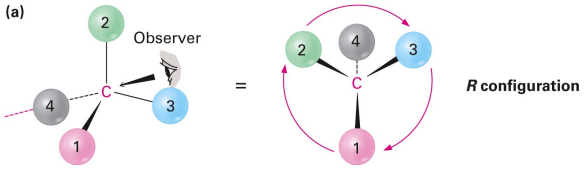
Cahn-Ingold-Prelog Priority Rules

Rule 1:

- Look at the four atoms (not group of atoms) directly attached to the chiral atom, and rank them according to atomic number, where 1 is the highest and 4 is the lowest priority.
- With the lowest priority group pointing away, look at the remaining 3 groups in a plane.
- From highest to lowest priority, clockwise is designated *R*, counterclockwise is designated *S*.

Is this *R* or *S*?

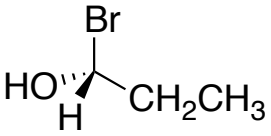


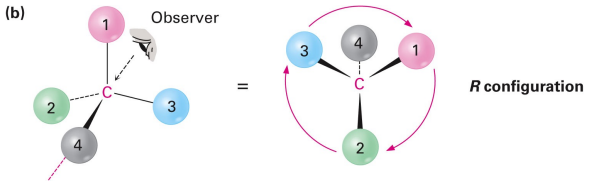


Rule 2:

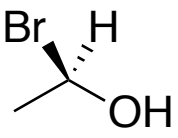
- If the lowest priority group is facing TOWARD you, rather than away from you, continue the standard method for determining *R* and *S*, but REVERSE the ending result. Alternatively, you can simply put your eye where it needs to be in order for the lowest priority group to be facing away from you - which is how the middle and right images are drawn, below.

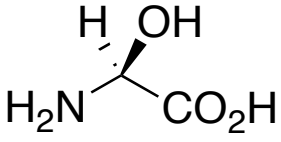
Is this *R* or *S*?

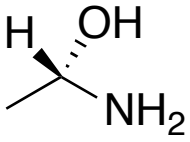




Assign *R* or *S* to the chiral carbons in each example:

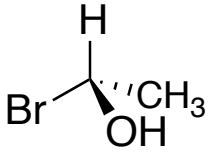


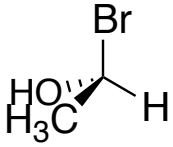




- If the lowest priority group is neither facing away from you or toward you (like below), adjust your perspective so it IS pointing away from you.

Assign *R* or *S* to the following:





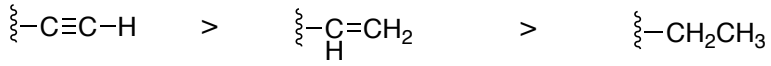
Rule 3:

- If a decision on priority cannot be reached by ranking the first atoms from the chiral atom, compare the second, third, or fourth atoms until a priority can be assigned.

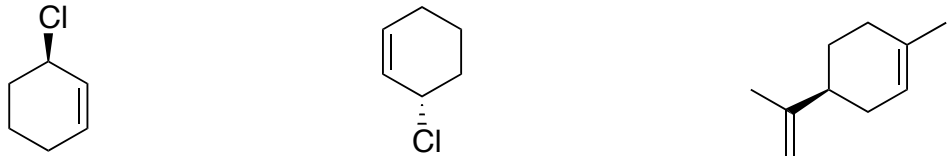
Which is (*R*)-2-chloropropane and which is (*S*)-2-chloropropane?

Rule 4:

- In most cases, it is safe to presume that atoms with a greater number of bonds are of a higher priority when compared to the *same* atom with less bonds, for example:

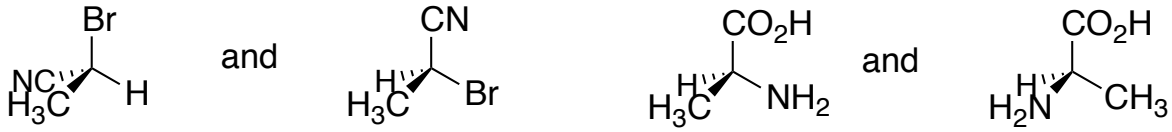


Try assigning the configuration of the chiral carbons below:



Let's Practice:

Assign (*R*) or (*S*) to the molecules below. Are the pairs the same or are they enantiomers?



Assign (*R*) or (*S*) configurations to the chiral carbons in the following isomer of menthol: