5.5: Simple Organic Enantiomers- R and S configurations

Stereochemistry is most important to us because of the role it plays in biology. Biological compounds usually belong to a class of compounds called organic compounds, originally meaning compounds that come from organisms. More generally, organic compounds contain carbon. because carbon is usually a tetrahedral atom, there is great potential for enantiomers in organic compounds, including biological ones.

The compound shown below contains a carbon connected to a hydrogen, a bromine, a chlorine and a fluorine. A tetrahedral atom connected to four different things is called a chiral center; it is a place where two different arrangements are possible.

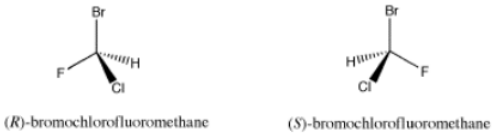


Figure 5.5.1: A pair of simple organic enantiomers.

This is not likely to be a naturally-occurring compound, although some marine organisms do make organic compounds containing bromine and chlorine. However, compounds similar to this one are sometimes used as general anaesthetics for surgical purposes. It is used as an example here because the chiral center is easy to see.

- A chiral center is a tetrahedral atom connected to four different groups.
- R and S configurations refer to the three-dimensional relationship of these groups around the chiral center.
- Assignment of R and S configuration follows a well-defined set of arbitrary rules. Anyone can follow these rules and arrive at the same configuration for the same structure.
- About half of S enantiomers rotate light in the (+) direction and about half rotate light in the (-) direction. R and S configurations do not correlate directly with optical rotation values; these are two ***unrelated*** systems for describing enantiomers.

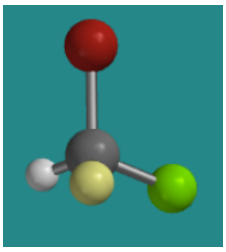


Figure 5.5.2: Ball-and-stick model of (*R*)-bromochlorofluoromethane.

Ball-and-stick model of bromochlorofluoromethane. Bromine is on top of the central carbon, fluorine points towards the camera, hydrogen is to the back left, chlorine is to the back right.

Go to **Animation SC4.1.** A three-dimensional model of (*R*)-bromochlorofluoromethane.

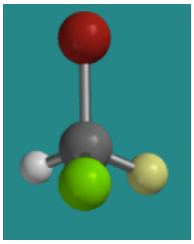


Figure 5.5.3: Ball-and-stick model of (*S*)-bromochlorofluoromethane.

Ball-and-stick model of bromochlorofluoromethane. Bromine is on top of the central carbon, chlorine points towards the camera, hydrogen is to the back left, fluorine is to the back right.

Go to **Animation SC4.2.** A three-dimensional model of (*S*)-bromochlorofluoromethane.

Rules for assigning *R* & *S* configuration:

- Find the chiral center(s).
- Compare the four atoms attached to the chiral center. What are their atomic numbers from highest to lowest?

- The highest atomic number has first priority; the second highest has second priority and so on.
- Turn the molecule so that the group with the lowest priority is away from you.
- Look at the three other groups. If they proceed in a clockwise direction from highest to second to third highest priority; the chiral center has the *R* configuration.
- If they proceed in a counterclockwise direction from highest to second to third highest priority; the chiral center has the *S* configuration.

Note

If two atoms connected to the chiral center have the same atomic number, you have to use a tie-breaker to decide which one gets higher priority. The tie-breaking rules are described on the next page; basically, you look at the next atoms attached to the ones that are the same.

Exercise 5.5.1

Explain the reasons for the assignment of configurations R and S in the models above. Assume red is bromine, bright green is chlorine and pale green is fluorine.

Answer

Priority of groups:

1 Br (red)

2 Cl (bright green)

3 F (pale green)

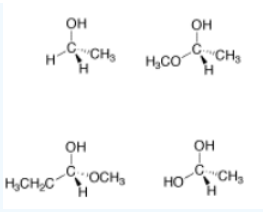
4 H (white)

In the molecule in Figure 5.5.2 (SC4.2), with the low-priority hydrogen pointed away, bromine is at the top, chlorine is clockwise from the bromine, and fluorine is clockwise from the chlorine. It therefore has an assigned configuration of *R*.

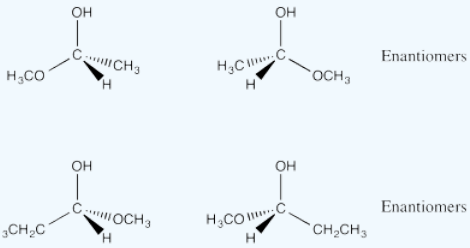
In the molecule in Figure 5.5.3 (SC4.3), with the low-priority hydrogen pointed away, bromine is at the top, chlorine is counterclockwise from the bromine, and fluorine is counterclockwise from the chlorine. Thus, it has an assigned configuration of *S*.

Exercise 5.5.2

Which of the following compounds have enantiomers? If they exist, draw them.



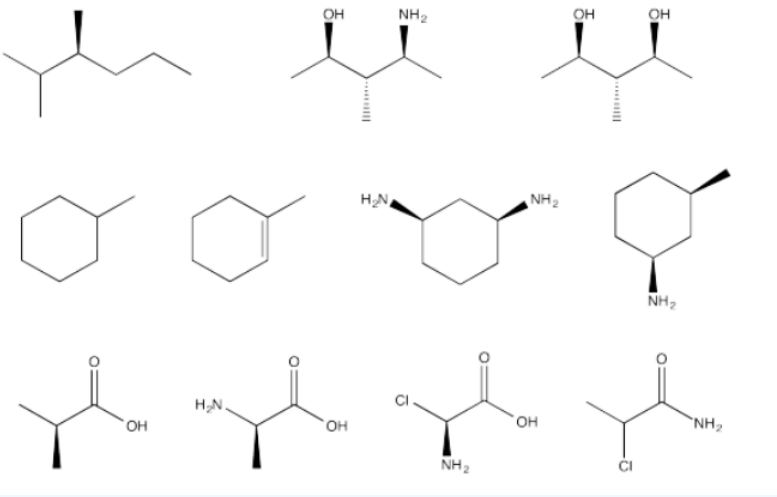
Answer



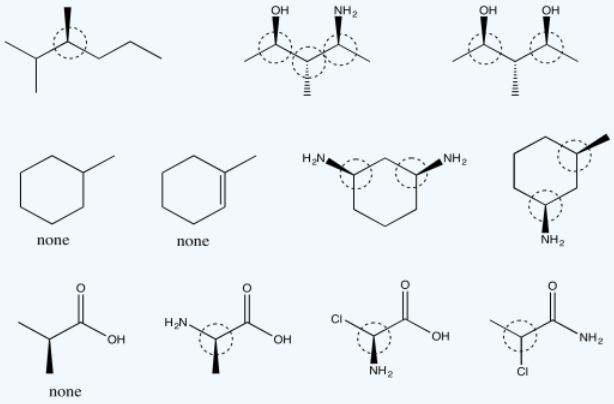
AnswerExercise 5.5.2, showing four different molecules with stereochemistry. Clockwise from top left: ethanol, 1-methoxy-1-ethanol, 1-ethoxy-1-propanol, 1,1-ethanediol.

Exercise 5.5.3

Circle the stereocenters in the following compounds.



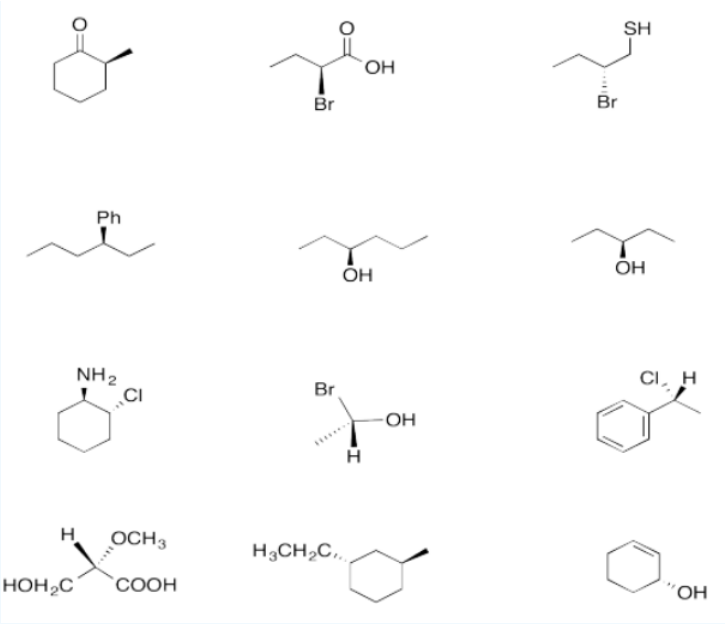
Answer



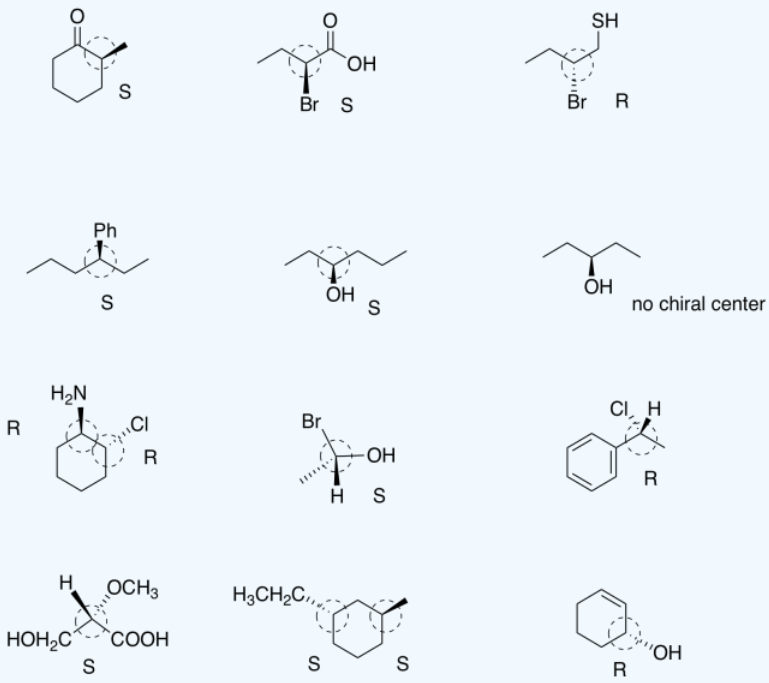
Answer

Exercise 5.5.4

Assign configuration of the stereocenters (*R* or *S*) in the following compounds.



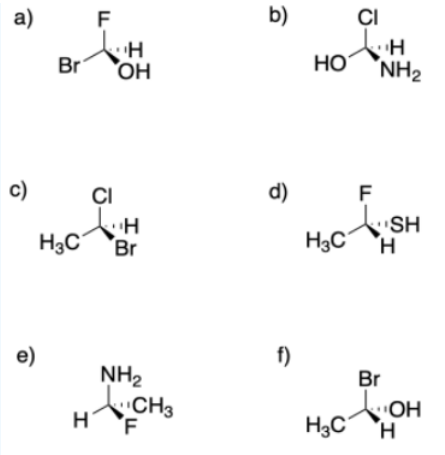
Answer



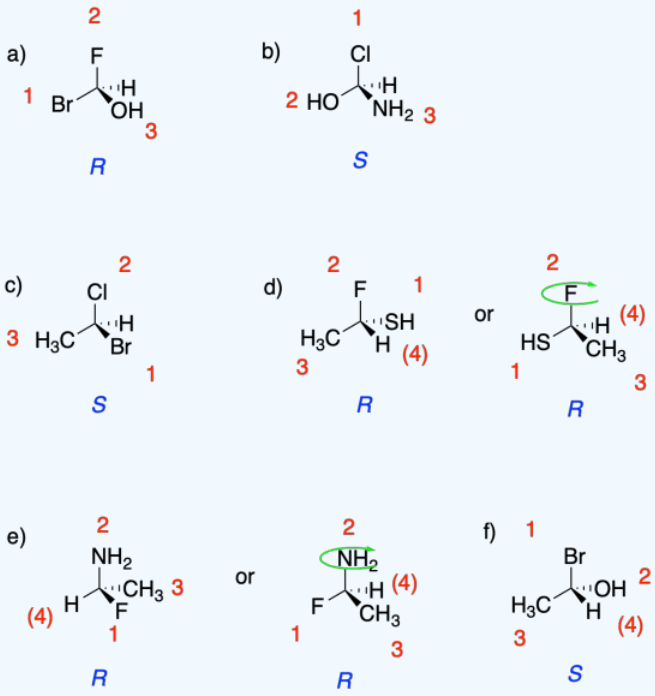
Answer

Exercise 5.5.5

Assign configurations (R or S) to the chiral centers in these molecules.



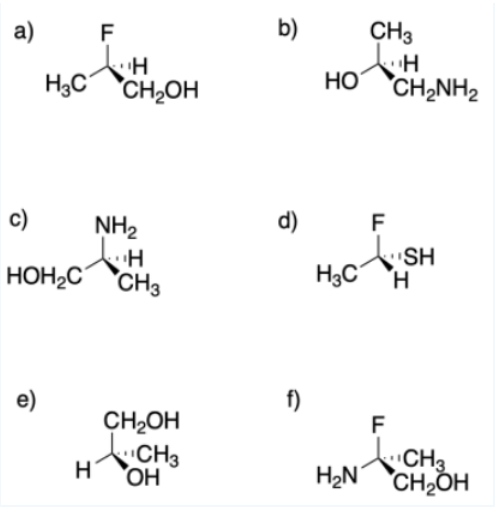
Answer



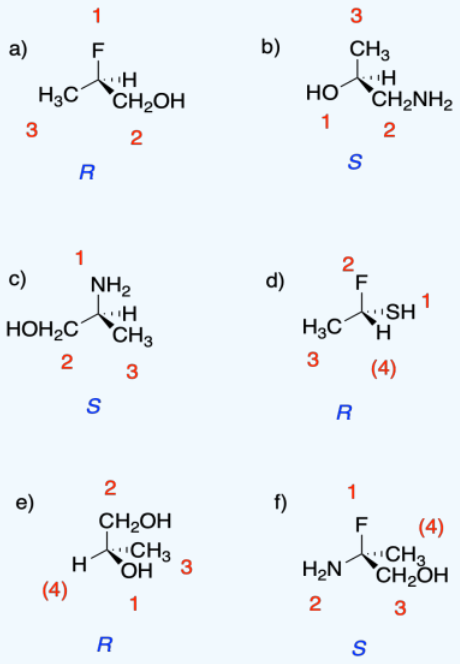
Answer

Exercise 5.5.6

Assign configurations (R or S) to the chiral centers in these molecules.



Answer



Answer