

STEREOCHEMISTRY

A STUDENT WHO HAS MASTERED THE MATERIAL IN THIS SECTION SHOULD BE ABLE TO:

1. Determine the relationship between two given structures (which may be any of the kinds below). Also, define each of the following terms, and give examples of pairs of molecules having the given relationship.

Same compound (superimposable or superposable)
Enantiomers (nonsuperimposable mirror images of each other)
Diastereomers (stereoisomers that are not mirror images of each other)
Stereoisomers (different orientation in space, same connectivity of atoms)
Constitutional Isomers (different connectivity of atoms; may include chain, position, and functional group isomers)

2. Define the following, and tell whether or not a given compound or structure fits the description or possesses the feature.

Chiral (not superposable on its mirror image), achiral
Tetrahedral stereocenter (chiral center)
Plane of symmetry
Optically active (rotates a plane of polarized light)
Meso compound (contains two or more stereocenters, but is achiral)

3. Given the structure, write the name, and given the name, draw the structure, of compounds using the (R)-(S) system (in addition to the IUPAC system you already know).
4. Define racemate (racemic mixture--equal and optically inactive mixture of a pair of enantiomers). Define the following, and calculate them given the appropriate information:

Specific rotation
Optical (enantiomeric) purity (enantiomeric excess)
Percent composition of optically impure samples

5. Predict the products of reactions, including their stereochemistry. Important reactions at this time (there will be many more later) are:

Reduction of alkyl halides
Halogenation of alkanes

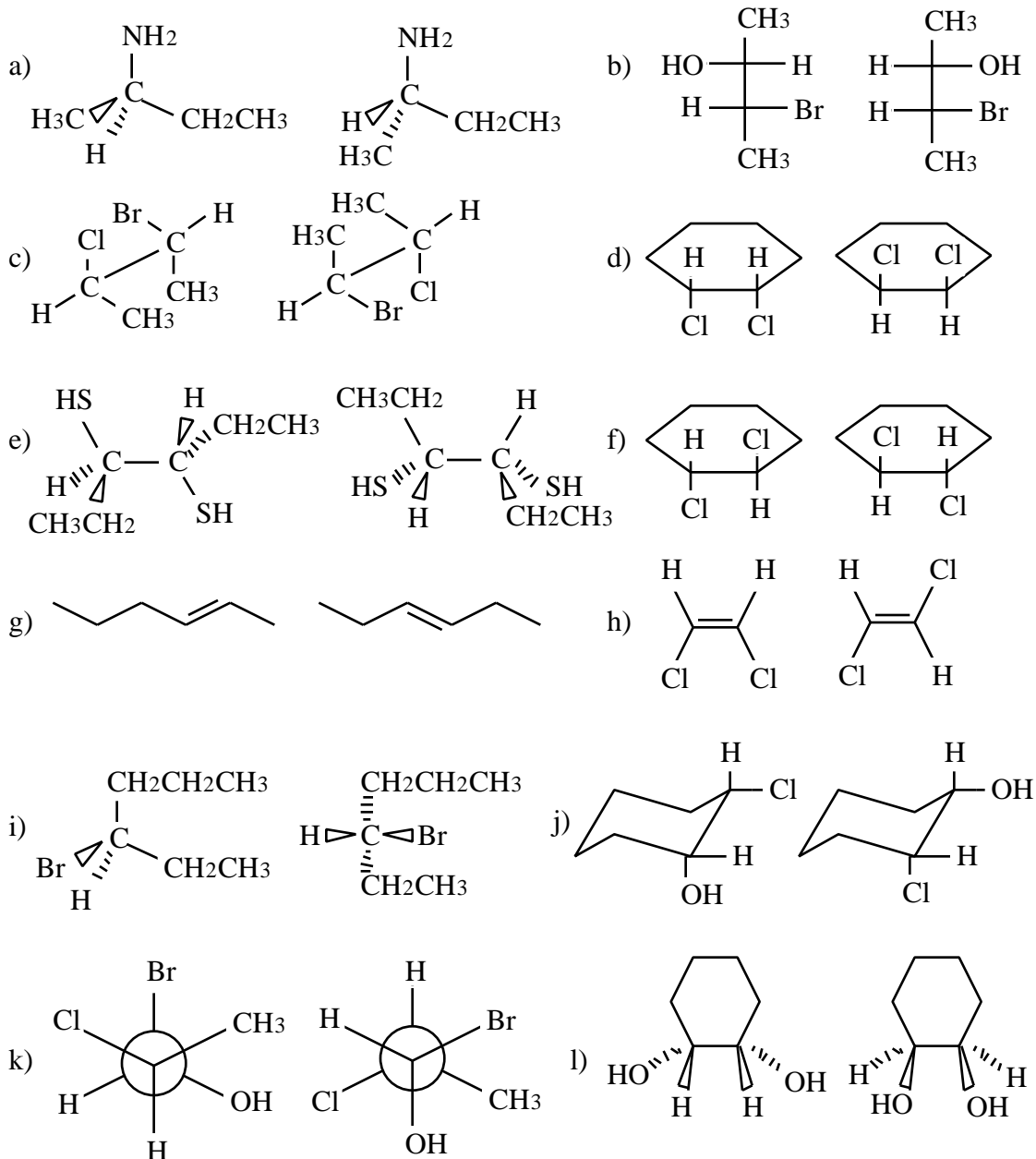
Important rules include (again, there will be more later):

When stereocenters are formed from achiral starting materials, the products are either achiral or formed as racemates (racemic mixtures).

When the starting material is chiral, and no bond to a stereocenter is broken or formed, retention of configuration occurs.

A STUDENT WHO HAS MASTERED THE OBJECTIVES ON THE PREVIOUS PAGE SHOULD BE ABLE TO SOLVE THE FOLLOWING PROBLEMS AND RELATED ONES:

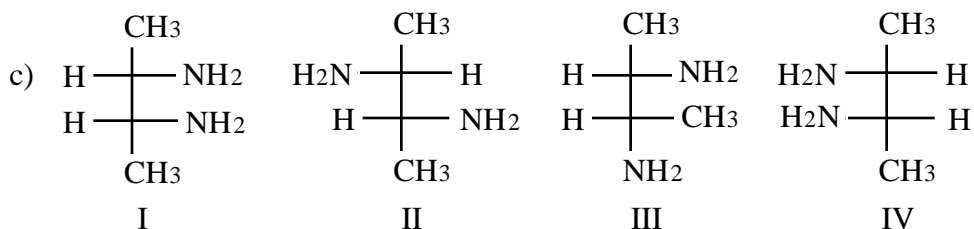
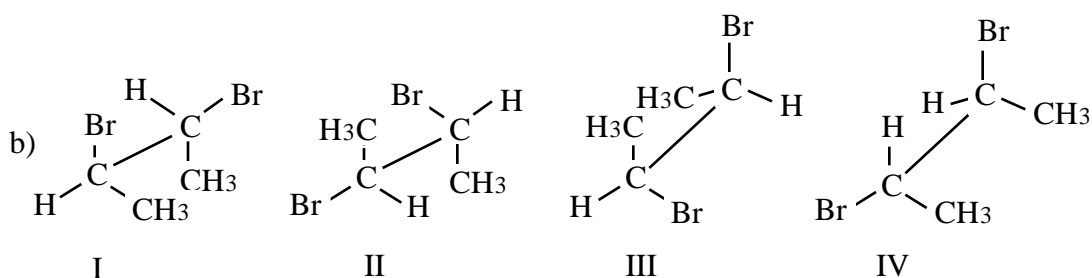
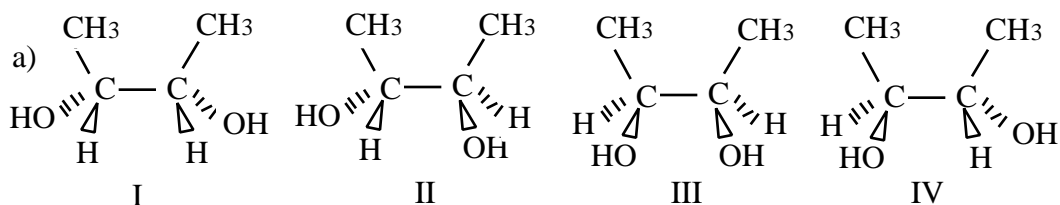
1.1 State how the two structures in each of the following pairs are related to each other. They may be constitutional (structural) isomers, enantiomers, diastereomers, or the same compound.



1.2 Identify each of the compounds in question 1.1 above as either chiral or achiral.

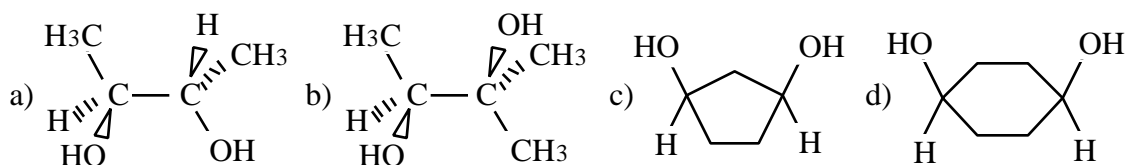
1.3 Answer the following questions for each of the following sets of four structures.

- 1) Which of the other three members of each set is not a stereoisomer of the first member of the set?
- 2) Which two members of each set are enantiomers of one another?
- 3) What relationship do the two members that are not enantiomers of one another have with the two that are enantiomers of one another? (See 1.1 for possible relationships.)

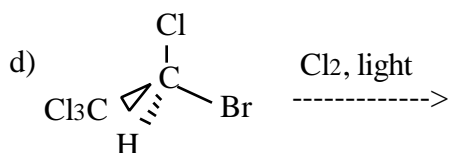
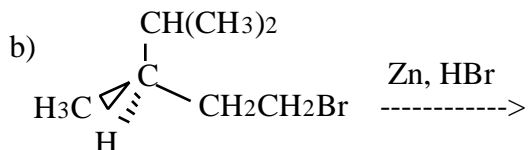
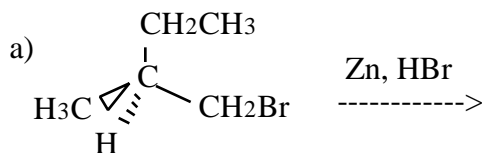


2.1 Answer the following questions for each of the molecules shown below.

- 1) How many tetrahedral stereocenters does the molecule contain?
- 2) Does the molecule possess any internal planes of symmetry?
- 3) Is the molecule chiral?
- 4) Is the molecule superposable on its own mirror image?
- 5) Is the molecule optically active?
- 6) Is this a meso compound?



5. Predict the products of each of the following reactions. (Note: When a product has more than one stereoisomer, your answer is not complete unless you indicate what stereoisomers are actually formed in the reaction. In answering this question, you must do that by drawing three-dimensional structures of all of the stereoisomers formed in the reaction, when appropriate.



ANSWERS TO THE PROBLEMS:

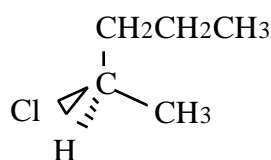
- 1.1 a) enantiomers b) diastereomers
 c) enantiomers d) same compound
 e) diastereomers f) enantiomers
 g) constitutional isomers h) diastereomers
 i) same compound j) enantiomers (hint: chairs can flip)
 k) diastereomers l) same
- 1.2 a) both are chiral b) both chiral, c) both chiral, d) both achiral, e) left structure achiral and right structure chiral, f) both chiral, g) both achiral, h) both achiral, i) both chiral, j) both chiral, k) both chiral, l) both achiral.
- 1.3
- | | | | |
|----|---------------|---------------|---------------|
| | a) | b) | c) |
| 1) | III | III | IV |
| 2) | II and IV | II and IV | II and III |
| 3) | diastereomers | diastereomers | diastereomers |
- 2.1
- | | | | | | | |
|----|----|-----|-----|-----|-----|-----|
| | 1) | 2) | 3) | 4) | 5) | 6) |
| a) | 2 | no | yes | no | yes | no |
| b) | 1 | no | yes | no | yes | no |
| c) | 2 | yes | no | yes | no | yes |
| d) | 0 | yes | no | yes | no | no |

2.2 6 tetrahedral stereocenters, $2^6 = 64$ possible stereoisomers

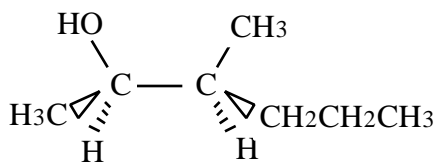
2.3 C

- 3.1 a) (S)-1-chloro-2-propanol
b) (S)-2-bromobutane
c) (2S,3S)-2,3-dichloropentane
d) (2S,3S)-2,3-butanediol

3.2 a) (R)-2-chloropentane



b) (2R,3S)-3-methyl-2-hexanol

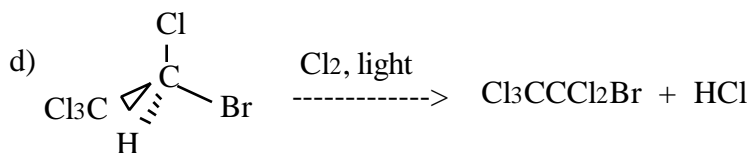
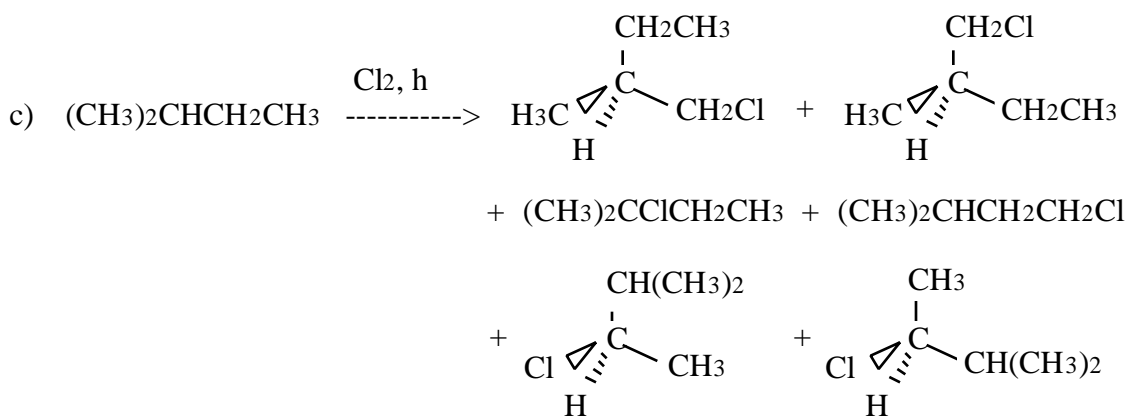
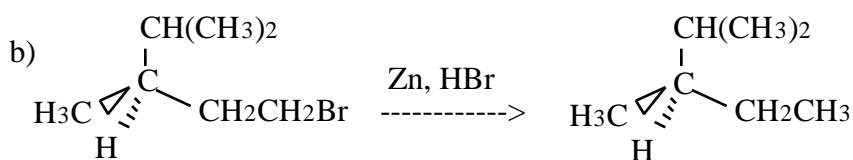


4.1 -41.5°

4.2 57.4 %

4.3 21.3% S and 78.7% R

5. Predict the products:



- 1) Consider the molecule at right, and answer each of the questions about it.
- a) Is it superimposable on its mirror image? _____

b) Is the molecule chiral? _____

c) Does it have a plane of symmetry? _____

d) Is it optically active? _____

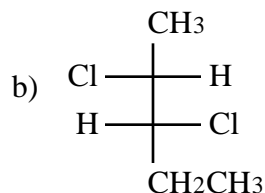
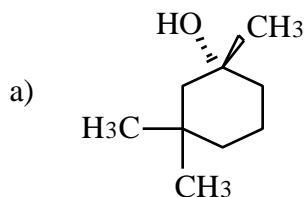
e) Is it a meso compound? _____
- 2) Give the IUPAC name of each, using R or S when appropriate.
- a)

b)
- 3) A sample of S-2-heptanol was found to have an optical purity of 30%. What is the percentage of racemic mixture of R and S-2-heptanol in this sample? Show your work.
- 4) What is the relationship between the structures in each of these pairs? Possible answers are Same compound, Enantiomers, Diastereomers, Constitutional (Structural) isomers. 4 ea.
- a)

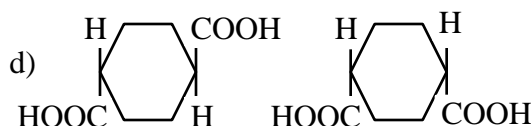
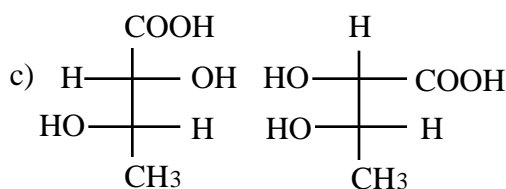
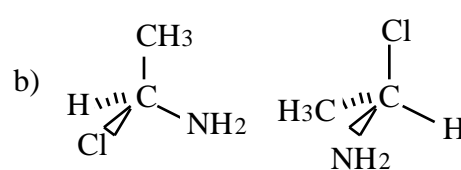
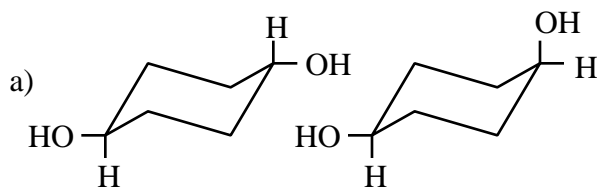
b)
- c)

d)
- e)
- 5) Predict the products of the reaction shown, indicating 3D structures when appropriate.
- $$\text{ClCH}_2\text{CH}_2\text{Cl} + \text{Br}_2 \xrightarrow{\text{LIGHT}} \text{-----}$$

1. Give the IUPAC name of each compound using R-S designation where appropriate.



2. What is the relationship between the structures in each of the following pairs? Possible answers are: same compound, enantiomers, diastereomers, constitutional isomers.



3. A sample of 3-(3,4-dihydroxyphenyl)alanine has a specific rotation of -4.5° . The specific rotation of optically pure $(-)$ -3-(3,4-dihydroxyphenyl)alanine is -11.5° .

a) What is the optical purity (enantiomeric excess) of the sample?

b) What is the percentage of $(+)$ -3-(3,4-dihydroxyphenyl)alanine in the sample?

4. Draw the structure of the chiral cyclic alkane having the lowest molecular mass. No isotopes are allowed.

5. Predict the organic products of the following reactions. Show three-dimensional structure where appropriate.

