

## 5.3: Stereochemistry - Extra Problems

### Optical rotation

#### Exercise 5.3.1

The (+) enantiomer of compound A has an optical rotation of  $125^\circ$ . If a pure sample of compound A has an optical rotation of  $100^\circ$ , what is the composition of the sample?

##### Answer

$$\text{Pure} = 125^\circ$$

$$\text{Optical purity} = \frac{100}{125} = 0.80$$

$$\%Major = 80 + \frac{20}{2} = 90\%$$

$$\%Minor = 100 - 90 = 10$$

#### Exercise 5.3.2

The (+) enantiomer of compound B has an optical rotation of  $100^\circ$ . If a pure sample of compound B has an optical rotation of  $95^\circ$ , what is the composition of the sample?

##### Answer

$$\text{Pure} = 100^\circ$$

$$\text{Optical purity} = \frac{95}{100} = 0.95$$

$$\%Major = 95 + \frac{5}{2} = 97.5\%$$

$$\%Minor = 100 - 97.5 = 2.5\%$$

#### Exercise 5.3.3

The (+) enantiomer of compound C has an optical rotation of  $18^\circ$ . If a pure sample of C contains 30% of the (+) enantiomer and 60% of the (-) enantiomer, what is the optical rotation value?

##### Answer

$$\text{Pure} = 18^\circ$$

$$\%Major = 60\%$$

$$\%Minor = 40\%$$

$$\text{Optical purity} = \frac{X}{18} = 20\%$$

Solve for X:

$$X = 3.6^\circ$$

#### Exercise 5.3.4

The (+) enantiomer of compound D has an optical rotation of  $25^\circ$ . If a pure sample of D contains 80% of the (+) enantiomer and 20% of the (-) enantiomer, what is the optical rotation value?

##### Answer

Pure =  $25^\circ$

$$\%Major = 80\%$$

$$\%Minor = 20\%$$

$$\text{Optical purity} = \frac{X}{25} = 80 - 20 = 60\%$$

Solve for X:

$$X = 15^\circ$$

## The polarimetry experiment

### Exercise 5.3.5

A pure sample of the naturally-occurring, chiral compound A (0.050 g) is dissolved in water (2.0 mL) and the solution is placed in a 0.5 dm cell. Three polarimetry readings are recorded with the sample:  $0.625^\circ$ ,  $0.706^\circ$ ,  $0.682^\circ$ . What is  $[\alpha]$ ?

**Answer**

$$[\alpha] = \frac{\text{observed rotation}}{(l)(c)}$$

$$c = \frac{0.050g}{2.0mL} = 0.025 \frac{g}{mL}$$

$$\text{Average observed rotation} = \frac{0.625 + 0.706 + 0.682}{3} = 0.671^\circ$$

$$[\alpha] = \frac{0.671^\circ}{(0.025 \frac{g}{mL})(0.5dm)} = 53.68^\circ$$

### Exercise 5.3.6

A pure sample of the chiral compound B (0.540 g) is dissolved in ether (2.0 mL) and the solution is placed in a 1.0 dm cell. Three polarimetry readings are recorded with the sample:  $1.225^\circ$ ,  $1.106^\circ$ ,  $1.182^\circ$ . What is  $[\alpha]$ ?

**Answer**

$$[\alpha] = \frac{\text{observed rotation}}{(l)(c)}$$

$$c = \frac{0.540g}{2.0mL} = 0.27 \frac{g}{mL}$$

$$\text{Average observed rotation} = \frac{1.225 + 1.106 + 1.182}{3} = 1.171^\circ$$

$$[\alpha] = \frac{1.171^\circ}{(0.27 \frac{g}{mL})(1.0dm)} = 4.34^\circ$$

### Exercise 5.3.7

A pure sample of the (+) enantiomer of compound C shows  $[\alpha] = 42^\circ$ . What would be the observed  $\alpha$  if a solution of the sample was made by dissolving 0.250 g in 2.0 mL of acetone and was then placed in a 0.5 dm cell?

**Answer**

$$[\alpha] = \frac{\text{observed rotation}}{(l)(c)}$$

$$c = \frac{0.250g}{2.0mL} = 0.125 \frac{g}{mL}$$

$$42^\circ = \frac{\text{observed rotation}}{(0.125 \frac{g}{mL})(0.5dm)}$$

observed rotation =  $2.625^\circ$

### Exercise 5.3.8

A student has prepared compound D in lab. She is sure the compound contains no impurities; a number of physical analyses have confirmed the structure and purity of the compound. A sample of compound D (0.10 g) is dissolved in methanol (2.0 mL) and the solution is placed in a 1.0 dm cell. Three polarimetry readings are recorded with the sample:  $0.995^\circ$ ,  $0.904^\circ$ ,  $0.936^\circ$ .

- What is  $[a]$ ?
- The optical rotation of D has previously been reported as  $25^\circ$ . What is the optical purity of this sample?
- What is the enantiomeric excess of this sample?
- What is the composition of this sample?
- Why did the previous analyses show that there was only one compound present?

#### Answer a

$$[a] = \frac{\text{observed rotation}}{(l)(c)}$$

$$c = \frac{0.10g}{2.0mL} = 0.05 \frac{g}{mL}$$

$$\text{Average observed rotation} = \frac{0.995 + 0.904 + 0.936}{3} = 0.945^\circ$$

$$[a] = \frac{0.945^\circ}{(0.05 \frac{g}{mL})(1.0dm)} = 18.9^\circ$$

#### Answer b

$$\% \text{ optical purity} = \frac{(100)(18.9)}{25} = 75.6\%$$

#### Answer c

$$\text{enantiomeric excess} = 75.6\%$$

#### Answer d

$$\frac{100 - 75.6}{2} = 12.2\%$$

12.2% one enantiomer

87.8% other enantiomer

#### Answer e

Enantiomers differ in how they interact with plane polarized light, but not in other physical analyses.

### Exercise 5.3.9

Suppose a student prepared a sample of a compound with known  $[a] = 40$ . The student did not realize that her sample contained 10% (by mass) of a non-chiral impurity. After correcting for  $c$  and  $l$ , what did she measure for  $[a]$ ?

#### Answer

$$[a] = \frac{\text{observed rotation}}{(l)(c)}$$

$$40^{\circ} = \frac{\text{observed rotation}}{(l)(c)}$$

$$40^{\circ} = \frac{\text{observed rotation}}{(l)(1.1c)}$$

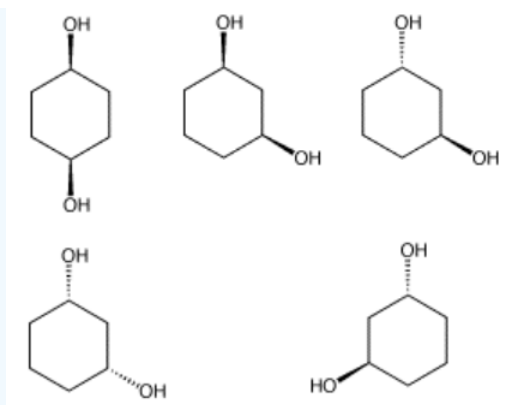
Observed rotation =  $44^{\circ}$

### diastereomers and physical properties

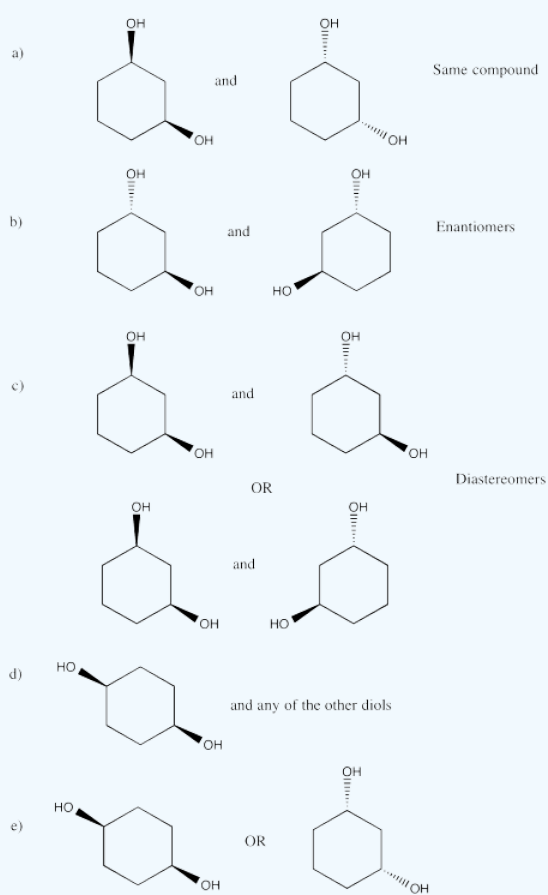
#### Exercise 5.3.10

From the following group of molecules, select:

- a pair that are the same compound.
- a pair that would have the same physical properties but opposite optical activities.
- a pair that have different physical properties but the same connectivity.
- a pair that have different connectivity.
- a compound that contains chiral centers but has no optical activity.



### Answer

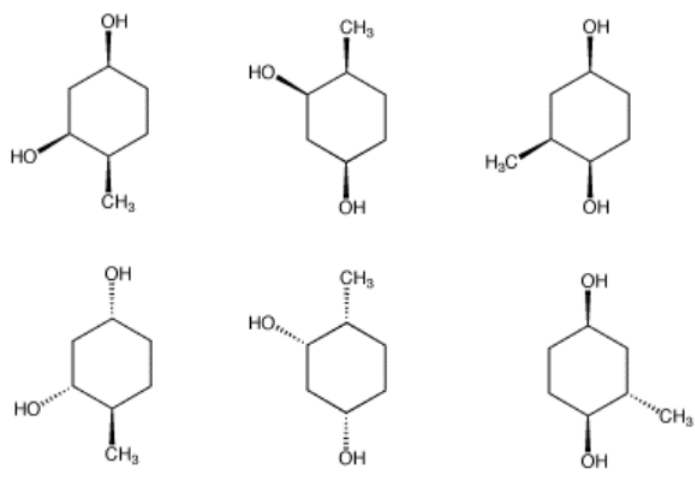


### Answer

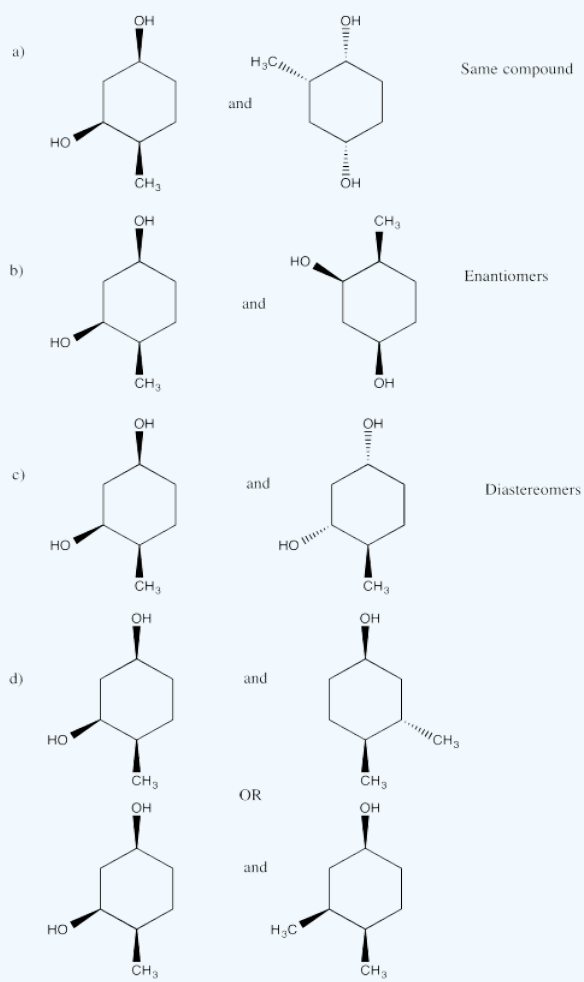
#### Exercise 5.3.11

From the following group of molecules, select:

- a pair that are the same compound.
- a pair that would have the same physical properties but opposite optical activities.
- a pair that have different physical properties but the same connectivity.
- a pair that have different connectivity.



### Answer

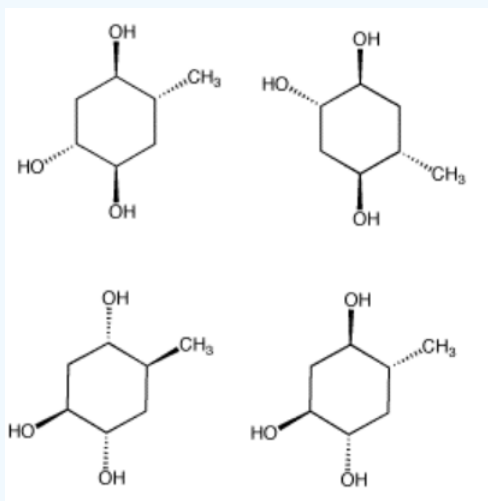


Answer

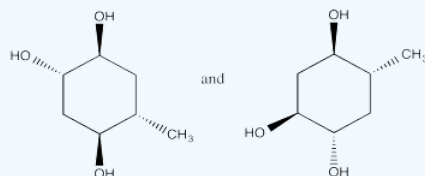
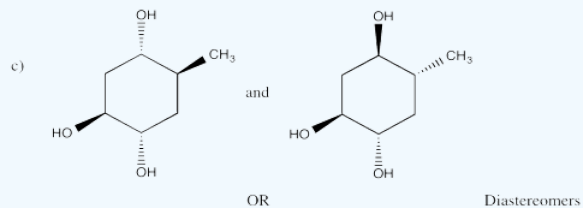
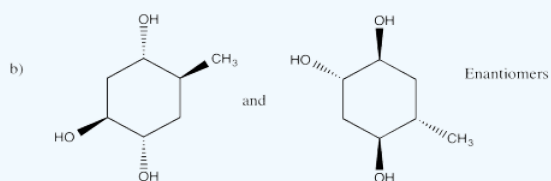
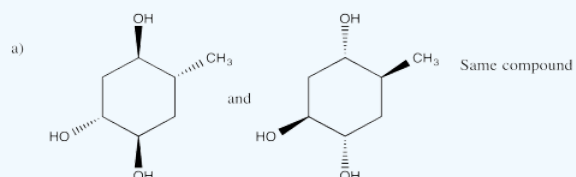
### Exercise 5.3.12

From the following group of molecules, select:

- a pair that are the same compound.
- a pair that would have the same physical properties but opposite optical activities.
- a pair that have different physical properties but the same connectivity.



### Answer



### Answer

Answers to Exercise 5.3.11, a through c. a is labelled "same compound". b is labelled "enantiomers". c is labelled "diastereomers".

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