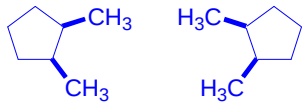
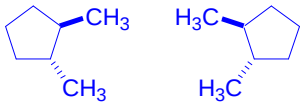
CHM 1321A
Assignment 3 Answers

1) Draw each structure below along with it's mirror image. Indicate whether the compound is chiral or achiral.

a) *cis*-1,2-dimethylcyclopentane. b) *trans*-1,2-dimethylcyclopentane

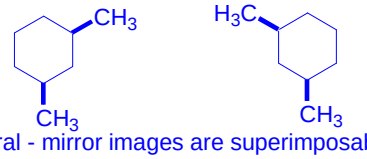
a) 

Achiral - mirror images are superimposable (meso compound)

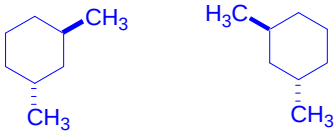
b) 

Chiral - mirror images are not superimposable

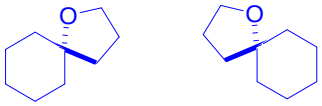
c) *cis*-1,3-dimethylcyclohexane d) *trans*-1,3-dimethylcyclohexane

c) 

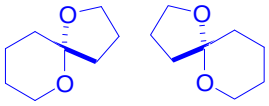
Achiral - mirror images are superimposable (meso compound)

d) 

Chiral - mirror images are not superimposable

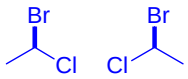
e) 

Achiral - mirror images are superimposable - no stereogenic centre, 2 identical groups on tetrasubstituted carbon

f) 

Chiral - mirror images are not superimposable

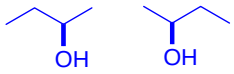
g) $CH_3CClBrH$ h) $(CH_3)_2CHOH$ i) $CH_3CH_2CHOHCH_3$ j)$CH_3CH_2CHOHCH_2CH_3$

g) 

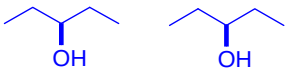
Chiral - mirror images not superimposable

h) 

Achiral - mirror images superimposable (2 identical groups on central carbon)

i) 

Chiral - mirror images not superimposable

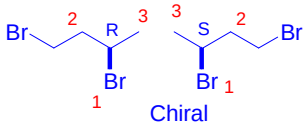
j) 

Achiral - mirror images superimposable (2 identical groups on central carbon)

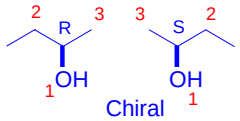
2) Draw the enantiomers of the following compounds and determine whether they are chiral. For all chiral compounds, determine whether each compound is R or S.

a) 1,3-dibromobutane b) 2-butanol c) 2-methylpentane d) 3-methylpentane
e) 3-methylhexane f) 1,2-dihydroxypropane g) 1, 2, 4-trihydroxybutane

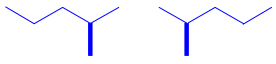
(Priorities in red)

a) 

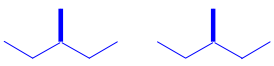
Chiral

b) 

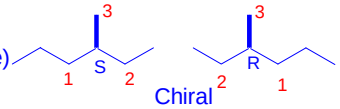
Chiral

c) 

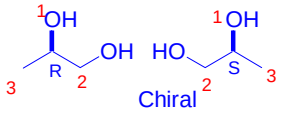
Achiral

d) 

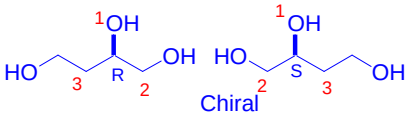
Achiral

e) 

Chiral

f) 

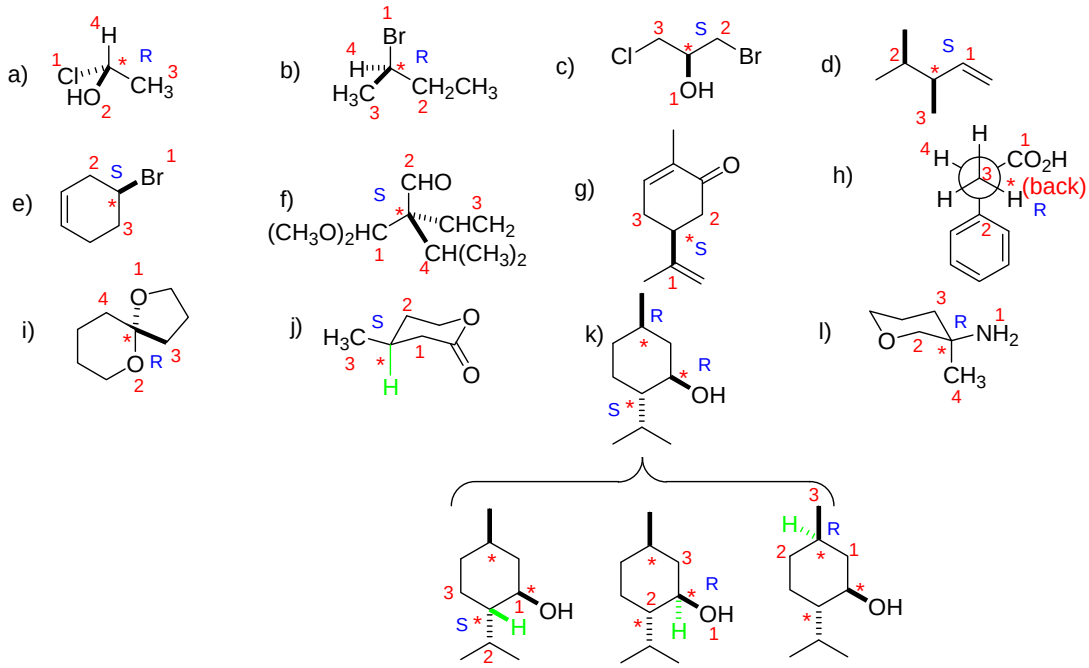
Chiral

g) 

Chiral

3) For the following compounds, show the stereogenic center(s) by labeling them with a star (*) and determine the configuration of each centre (R or S).

(Priorities in red - if no 4th group is shown, it is the implied hydrogen, hydrogens in green have been added)



4) A solution of 2.0 g of (+)-glyceraldehyde in 10mL of water was placed in a 100 mm cell. Using the sodium D line, a rotation of +1.74° was found. Determine the specific rotation of (+)-glyceraldehyde.

$$[\alpha]_D = \frac{100 \bullet \alpha}{l \bullet c}$$

$$c = \frac{2.0\ g}{10\ mL} \times \frac{100\ mL}{1 \times (100\ mL)}$$

this is the unit!

c = 20 g/100mL

$$l = 100\ mm \times \frac{1\ dm}{100\ mm} = 1\ dm$$

$$[\alpha]_D = \frac{100\ (+1.74)^{o}}{20 \bullet 1} = +8.7^{o}$$

5) A solution of 0.5 g of (-)-epinephrine dissolved in 10 mL of dilute HCl was placed in a 20 cm polarimeter tube. Using the sodium D line, the rotation was found to be -0.5° at 25 °C. Determine the specific rotation of (-)-epinephrine.

$$[\alpha]_D^{25} = \frac{100 \bullet \alpha}{l \bullet c}$$

$$c = \frac{0.5\ g}{10\ mL} \times \frac{100\ mL}{1 \times (100\ mL)}$$

this is the unit!

c = 5.0 g/(100mL)

$$l = 20\ cm \times \frac{1\ dm}{10\ cm} = 2\ dm$$

$$[\alpha]_D^{25} = \frac{100(-0.5)^{o}}{5.0 \bullet 2} = -5.0^{o}$$

6) A chiral sample gives a rotation that is 180°. Describe how you would determine whether the rotation was +180° or -180°.

Lower the concentration. This will decrease the magnitude of the rotation allowing the sign to be determined

7) Calculate the ee and specific rotation of a mixture containing 6 g of (+)-glucose and 4 g of (-)-glucose. The specific rotation of pure (-)-glucose is -17.6°.

$$ee = \frac{|d - l|}{d + l} \times 100$$

d = 6 g
l = 4 g (remember that d isomer has + rotation)

$$ee = \frac{|6\text{ g} - 4\text{ g}|}{6\text{ g} + 4\text{ g}} \times 100$$

ee = 20%

$$\text{optical purity} = ee = \frac{\text{specific rotation of mixture}}{\text{specific rotation of pure}} \times 100$$

$$.2 = \frac{\text{specific rotation of mixture}}{17.6}$$

specific rotation of mixture = 3.52^{o}

since the (+) isomer is in excess, the sign of the rotation will be positive

specific rotation of mixture = $+3.52^{o}$

8) A 0.05g sample is dissolved in 2.0 mL of $CHCl_3$. When placed in a 2.0 cm polarimeter tube, the observed clockwise rotation was 0.043°. Calculate the specific rotation of the sample.

$$[\alpha]_D = \frac{100 \bullet \alpha}{l \bullet c} \qquad c = \frac{0.05\text{ g}}{2\text{ mL}} \times \frac{100\text{ mL}}{1 \times (100\text{ mL})}$$

c = 2.5 g/100mL

$$l = 2\text{ cm} \times \frac{1\text{ dm}}{10\text{ cm}} = 0.2\text{ dm}$$

$$[\alpha]_D = \frac{100(+0.043)^{o}}{2.5 \bullet 0.2} = +8.6^{o}$$

9) (-)-Lactic acid has a specific rotation of -12.3°. Calculate the specific rotation of a mixture of 64% (+)-lactic acid and 36% (-)-lactic acid.

$$ee = \frac{|d - l|}{d + l} \times 100 = \text{optical purity}$$

d = 64
l = 36

$$ee = \frac{|64 - 36|}{64+36} \times 100$$

ee = 28% = optical purity

$$\text{optical purity} = \frac{\text{specific rotation of mixture}}{\text{specific rotation of pure}} \times 100$$

$$0.28 = \frac{\text{specific rotation of mixture}}{12.3}$$

specific rotation of mixture = 3.44^{o}

10) The specific rotation of pure (S)-phenylalanine is +16.4°. A sample of phenylalanine has a specific rotation of -10.4°.

a) What is the ee of the sample?

ee = optical purity = 10.4°/16.4°X100%

= 63.4 %

b) What is the predominant isomer in the mixture?

Since the rotation is negative, the (R) isomer must be predominant

c) What is the ratio of isomers in the solution?

$$ee = \frac{|d - l|}{d + l} X100$$

$d + l = 100$

$d = 100 - l$

$$ee = \frac{|100 - 2l|}{100} X100$$

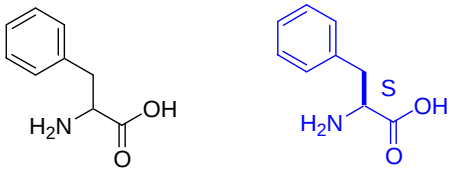
$63.4 = 100 - 2l$

$$l = \frac{63.4-100}{-2}$$

$l = 18.3$ and $d = 81.7$

Ratio = 81.7/18.3 = 4.46 : 1

d) Phenylalanine has the following structure, given that the configuration or natural phenylalanine is S, what is the proper way to draw phenylalanine in its naturally occurring form?

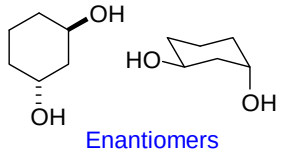


11) Give the stereochemical relationship between each pair of isomers (enantiomers, diastereomers, meso compounds). (If you have trouble with this question, try using models)

a)

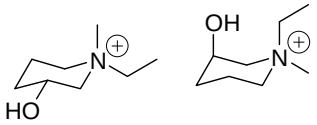
Enantiomers

b)



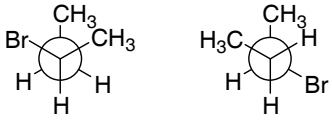
Enantiomers

c)



Same Compound

d)



Same Compound