1. A new drug called *Weloveochem* is being tested for its enantiomeric purity in the labs. The enantiopure specific rotation of (-)-*Weloveochem* at 25° C is known to be -38° ([α]_D^{25}).

a. What is the observed rotation for a solution of *Weloveochem* containing 0.96 g (+)-*Weloveochem* and 0.01 g (-)-*Weloveochem* in 100 mL of solvent? Assume a 1 dm cell.

Find concentration: 

\[
\text{Concentration} = \frac{0.96 \text{ g (+)-*
Weloveochem* - 0.01 g (-)-*
Weloveochem*}}{100 \text{ mL}} = 0.95 \text{ g mL}^{-1}
\]

\[
\alpha = [\alpha]_{\text{cl}}, \text{ where } \alpha = \text{observed rotation, [} \alpha\text{]} = \text{specific rotation}, \text{ c = concentration in (g/mL), and l = length of cell in dm}
\]

\[
\alpha = (38^\circ)(\frac{0.95 \text{ g}}{100 \text{ mL}})(1 \text{ dm}) = 0.361^\circ
\]

b. If a solution has a specific rotation of -9.8°, what is the stereochemical composition (% (-)-*Weloveochem* and (+)-*Weloveochem*) of this mixture?

Calculate %ee

\[
\%\text{ee} = \frac{\text{measured sp. rotation of mixture}}{\text{measured sp. rotation of pure enantiomer}} \times 100
\]

\[
\%\text{ee} = \frac{-9.8}{-38.0} \times 100 = 25.8\% \text{ enantiomeric excess}
\]

Determine (+) and (-) composition of enantiomeric excess

25.8% (-)-enantiomer means that there is 74.2% of the mixture that is an equal mix of 37.1% (-)-*Weloveochem* and 37.1% (-)-*Weloveochem*

So, the total % (-)-*Weloveochem* = 25.8% + 37.1% = 62.9%

the total % (+)-*Weloveochem* = 37.1%

c. What is the specific rotation of (+)-*Weloveochem*?

Remember that (-)-*Weloveochem* and (+)-*Weloveochem* are enantiomers. Their specific optical rotations will be equal in magnitude but opposite in sign. So the specific enantiomeric rotation of (+)-*Weloveochem* would be +38.0°.
Remember that this also means that if you have an equimolar mixture of the (+) and (-) enantiomer, your observed optical rotation would be 0.

d. If you dissolve 0.5 g of (-)-Weloveochem in 100 mL of water, what would the specific rotation of (-)-Weloveochem be in this mixture? Assume a 1 dm cell. The specific rotation of one enantiomer of a chiral compound will not change due to changes in concentration. Only the observed optical rotation of the mixture will change with changes in concentration.

The specific rotation of (-)-Weloveochem will always be -38° as outlined by the original question.

e. What if you doubled the amount of water in the solution from part D? What would the specific rotation of (-)-Weloveochem be in this mixture? The specific rotation of one enantiomer of a chiral compound will not change due to changes in concentration. Only the observed optical rotation of the mixture will change with changes in concentration.

The specific rotation of (-)-Weloveochem will always be -38° as outlined by the original question.

f. What would the observed angle of rotation of the mixture be in the solution from part E?

Find concentration from part E:

\[
\text{Concentration} = \frac{0.50 \text{ g}}{200 \text{ mL}}
\]

\[\alpha = (\text{specific rotation of pure chiral compound}) \times (\text{concentration}) \times (\text{diameter of cell})\]

\[\alpha = (-38°) \left( \frac{0.50 \text{ g}}{200 \text{ mL}} \right)(1 \text{ dm})\]

\[\alpha = -0.095°\]

**alternatively you can find the observed optical rotation using part F’s concentration and half your final answer**
2. Suppose a drug is known to work best only when it is the pure chiral compound. As a member of the lab that is testing the effects of this new drug, you are asked to find the specific rotation of the enantiopure drug, but you only have at hand a solution that is 90% of the (+)-enantiomer and 10% of the (-)-enantiomer. You measure the observed rotation of this solution to be 17.3°. What is the specific rotation of a solution of pure (-)-enantiomer of this drug?

Write down your givens:
- We know from the problem that there is 80% enantiomeric excess (90% - 10%)
- We know that the specific rotation of the mixture is measured to be 17.3°

So, we can use this equation to solve for the pure optical rotation

\[
\text{%ee} = \frac{\text{measured sp. rotation of mixture}}{\text{measured sp. rotation of pure enantiomer}}
\]

\[
0.80 = \frac{17.3°}{\text{measured sp. rotation of pure enantiomer}}
\]

Specific rotation of pure (+) enantiomer = 21.6° so specific rotation of pure (-) enantiomer is -21.6°

3. The following questions refer to the molecules below:

(a) What is the relationship between these two molecules?
   (i) They are enantiomers.

(b) Which is the S enantiomer and which is the R enantiomer?
   (i) The one on the left is the S enantiomer and the one on the right is the R enantiomer.

(c) What are the IUPAC names of these molecules?
   (i) Left: (S)-2-chlorobutane and right: (R)-2-chlorobutane
   Show students how to redraw them with the ethyls drawn out to easier determine the IUPAC name

(d) Which of the following traits would differ between these two molecules?
   (i) Boiling point? no
   (ii) Specific optical rotations? yes
   (iii) Density? no
   (iv) Dipole moment? no
   (v) Solubility in a chiral compound? yes
4. The following questions refers to the following molecule:

(a) Draw all stereoisomers of this molecule and label them as diastereomers or enantiomers. Label all stereocenters as S or R. (note: a problem like is harder than what will be on Midterm 2, but knowing the relationships between two given stereoisomers is very important!)

1 and 2 are enantiomers
3 and 4 are enantiomers
1+3, 1+4, 2+3, 2+4 are all diastereomers.

(b) Draw all the highest energy newman projection of the original molecule, label it as staggered/gauche, staggered/anti, or eclipsed.
    (i) For extra practice: draw all 6 Newman projections of the molecule.

**answer**
5. a) Rank the following compounds by increasing Intermolecular Forces (IMFs).

a) ClCH₂COOH   

b) 

c) 

d) NH₂CH₂COOH  

e) 

b)  

c)  

e)  

a)  

d)  

Compound B only has van-der-waals interactions.

Compound C has van-der-waals interactions and dipole-dipole interactions.

Compound E has van-der-waals interactions and dipole-dipole interactions. The 2 fluorines on one end of the molecule create stronger dipoles than the single fluorine in compound C.

Compound A has van-der-waals interactions, dipole-dipole interactions, and hydrogen bonding.

Compound D has van-der-waals interactions, dipole-dipole interactions, and hydrogen bonding at 2 sites in the molecule.

Indicate which molecules are capable of hydrogen bonding with H₂O.

A, C, D, E, are capable of H-bonding with water.

6. Draw the following compound in 2 chair conformations and determine which is more stable. Write a 1 sentence explanation for why.

The first conformation is more stable because the large isopropyl group is in the equatorial position, which minimizes steric hindrance created by the substituents on the ring.

7. Identify stereocenters in the following molecule.
b) Determine how many possible stereoisomers there are for the molecule. 
\[ 2^3 = 8 \text{ potential stereoisomers} \]

8. Draw all the possible stereoisomers for the following compounds and determine the relationship between them. Make sure to label each stereocenter as S or R.

a) 

Drawing the mirror image of the molecule shows that the 2 are identical. This molecule is achiral and meso (it is achiral and has tetrahedral stereocenters)

b) (Note: Dr. King will most likely not ask you to draw out so many stereoisomers, but knowing the slight differences between enantiomers and identical molecules is very important.)

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<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<tr>
<td>(R,R)</td>
<td>(S,S)</td>
<td>(S,R)</td>
<td>(R,S)</td>
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1 is the original molecule
2 is the mirror image of the original molecule.
3 is a diastereomer to the original molecule - molecules of the same formula with 2 or more stereocenters that are not mirror images of each other
4 is the mirror image of 3.

Relationships:
1&2 are enantiomers - non superimposable mirror images.
   For enantiomers - switch conformation at both stereocenters.
1&3, 1&4, 2&3, 2&4 are diastereomers
   For diastereomers - switch conformation at one stereocenter only.
3&4 are IDENTICAL - if you flip over 4, you get the same molecule as 1 because both stereocenters have the same substitutions.

9. Given the following energy diagram for the reaction below:

\[
\begin{align*}
\text{X} & \quad \text{Y} \\
\rightarrow & \\
\text{X}^\ominus & \quad \text{Y}^\ominus
\end{align*}
\]

a) Label the activation energy and the change in enthalpy of the reaction. (below)

b) Determine whether the reaction is endothermic or exothermic.

   Endothermic - the products are at a higher energy than the reactants.

c) Is this cleavage heterolytic or homolytic?

   Heterolytic - electrons were unequally distributed to the 2 products.

d) Draw the transition state of the reaction.

   \[
   \delta^- \quad \delta^+ \\
   \mid \text{X} \ldots \text{Y} \mid^\ddagger
   \]

   There is a partial negative on X and a partial positive on Y.

e) Which component of the energy diagram would a catalyst most likely change?

A catalyst would most likely affect activation energy, by lowering it to make the reaction proceed faster.

10. Rank the following cycloalkenes in order of stability:

   a. 

   ![Cycloalkenes](image)
11. Convert the following molecule to a chair conformation, perform a chair flip, and indicate which of the conformations predominates in an equilibrium mixture at room temperature. Give a 1 sentence explanation for your choice.

The chair conformation on the right contains both substituents in the equatorial position instead of the axial position and this di-equatorial is a more stable conformer and predominates the equilibrium mixture at room temperature.

12. True/False. Give a 1-sentence explanation for each statement.

b. (T/F) Stereoisomers are compounds that have the same molecular formula but different atom connectivity
   i. Explanation: Stereoisomers are compounds that have the same atom connectivity but different arrangement of atoms in space.

   c. (T/F) If the mirror image of a molecule is superimposable on the original molecule, then these molecules are identical.
   i. Explanation: The mirror image if superimposable can be rotated in order to match the original molecule, making it them identical and achiral.
d. (T/F) Any molecule that is not superimposable on its mirror image is achiral.
   i. Explanation: Any molecules that cannot be superimposed on its mirror image is chiral.

![Non-superimposable Mirror Images](image)

![Molecules which are not superimposable on their mirror images are called enantiomers.](image)

e. (T/F) Chiral molecules always have planes of symmetry.
   i. Explanation: Chiral molecules do not have planes of symmetry. If you can find a plane of symmetry, then it is superimposable on its mirror image and is achiral.

f. (T/F) Molecules with more than one stereocenter are always chiral.
   i. Explanation: If a molecule has only one stereocenter then it is always chiral. However, if it has two or more, then the molecules can be chiral or achiral.

13. Label the stereocenters, if any, in the following molecules: (Note: a problem like part H has more stereocenters than you will see on a problem on Midterm 2, but is still good practice for identifying stereocenters!)

g. ![Molecule](image)

h. ![Molecule](image)
14. Label the following pairings of molecules as identical/enantiomers *look out for diastereomer relationships on Midterm 2 also!*

i. 

![Image of a molecule with the label "Identical"]

Identical

j. 

![Image of two molecules with the label "Enantiomers"]

Enantiomers

k. 

![Image of four molecules with the label "Enantiomers"]

Enantiomers
1. identical