MIDTERM 2 REVIEW KEY

Key Concepts:
- Newman projections
  - Both anti and gauche staggered conformations, eclipsed conformation
  - Stability of different conformations, know how to draw energy diagrams
- Effect of branching in boiling points for alkanes
- Chair conformation
  - Know how to draw a flipped chair
  - Stable chairs have substituents in the equatorial position
- Differentiate between constitutional isomers, stereoisomers, identical molecules and neither
- Assign R and S configuration
- Differentiate between enantiomers, diastereomers and meso compounds

Chapter 4

1. Rank the group of alkanes in order of increasing boiling point. Explain your choice of order.
   a. CH₃CH₂CH₂CH(CH₃)₂, CH₃(CH₂)₄CH₃, (CH₃)₂CHCH(CH₃)₂
      i. CH₃(CH₂)₄CH₃ > CH₃CH₂CH₂CH(CH₃)₂ > (CH₃)₂CHCH(CH₃)₂
         with CH₃(CH₂)₄CH₃ as the highest boiling point since it has the least branching.
         Since alkanes only exhibit van der waals (VDW) force, the greater the surface area the molecule has the stronger VDW and higher the boiling point. Alkanes with many substituents branching off from its parent chain disrupts the surface area and thus decrease the VDW and boiling point.
2. Consider rotation around the carbon-carbon bond in 1,2-dichloroethane (ClCH₂CH₂Cl).
   a. Using Newman projections, draw all of the staggered and eclipsed conformations that result from rotation around this bond.

   i. When rotating, ONLY rotate the front or back carbon. Do not rotate both front and back carbons at once! When you are asked to draw all staggered and eclipsed projections, there should always be a total of 6 Newman projections (360 degrees / 60 degrees = 6) in the end. For eclipsed conformations, the substituents from front and back carbon should be directly on top of each other while in a staggered conformation, the substituents are facing opposite directions.
b. Graph energy versus dihedral angle for rotation around this bond.

i. The staggered, anti conformation will have the lowest energy since it’s the most stable conformation, with the biggest Cl groups facing 180 degrees away and the all the hydrogens are equally spaced out. The eclipsed conformation with two Cl groups overlapping with one another (conformation 4) will have the highest energy due to both torsional and steric stains.
3. For each compound drawn below:

   1
   2
   3

   a. Draw the two possible chair conformations for the cis isomer. Which conformation, if either is more stable?

   i.  

   ii. 

   iii.
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b. Draw the two possible chair conformations for the trans isomer. Which conformation, if either, is more stable?

![Conformation 1](image1.png)

i.

![Conformation 2](image2.png)

ii.

![Conformation 3](image3.png)

iii.

c. Which isomer, cis or trans, is more stable and why?

i. For structure 1, the cis isomer will be more stable than the trans isomer since cis isomer has both groups in equatorial position. For structures 2 and 3, the trans isomer will be most stable because it has both groups in equatorial position.
4. Classify each pair of compounds as constitutional isomers, stereoisomers, identical isomers, or not isomers of each other.

a. i. Stereoisomers, the conformation on the left is trans while the conformation on the right is cis isomer.

b. i. Identical.

c. i. Not isomers. The structure on the left has a molecular formula of C₆H₁₀ and the structure on the right has a molecular formula of C₆H₁₂.
5. Classify each pair of compounds as constitutional isomers or identical molecules.

a. i. Identical.

3-ethyl-2-methylpentane

3-ethyl-2-methylpentane
b. i. Constitutional isomers
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Chapter 5

6. Give the IUPAC name for each compound, including the R,S designation for each stereogenic center.

To make the IUPAC name, start by finding the longest carbon chain. Then number the chain such that you can give the substituents the lowest number possible. To determine the R and S designations recall that larger atomic number atoms are given priority. So, number each substituent on a chiral carbon by giving the largest atomic number the priority. Once that is established, follow the 1→4 designation. If it is clockwise, it is R and counterclockwise is S. Note that if a Hydrogen is on a wedge, use the same steps mentioned above but give the opposite designation in the end.

a.

\[
\begin{array}{cccccc}
9 & 7 & 5 & 3 & 1 \\
10 & & & & & \\
\end{array}
\]

\textit{(4R,6R)-4-ethyl-6-methyldecane}

b.

\[
\begin{array}{cccc}
6R & 5S & 3R \\
9 & 7 & 1 \\
\end{array}
\]

\textit{(3R,5S,6R)-5-isobutyl-3,6-dimethylnonane}
8. Locate the stereogenic centers.

Recall that stereogenic centers are carbons that have 4 different groups bonded to it. Be sure to draw all Hydrogens that are bonded to the carbons since they count as well when determining the groups.

![Chemical structure of amoxicillin](image)

9. How are the compounds in each pair related to each other? Are they identical, enantiomers, diastereomers, constitutional isomers, or not isomers of each other?

Enantiomers are compounds that are mirror images and are not superimposable. Another way to think of them is that they have complete opposite R and S designations. Diastereomers differ in at least one but not all stereocenters.

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10. Which group in each pair is assigned the higher priority in R,S nomenclature?

To determine which has higher priority, determine which atom has the higher atomic number. If they have the same atomic number, look at which has a greater mass. If they have the same atom, look at the atom bonded to the first one in each group and determine either the greater atomic number or mass for that atom.

a. –OH, –NH₂
b. –CD₃, –CH₃
c. –CHO, –COOH

11. Label each stereocenter as R or S

To assign R or S to the molecule, first rank the groups. The lowest priority group must be oriented behind the page. If tracing a circle from (1) → (2) → (3) proceeds in the clockwise direction, the stereogenic center is labeled R; if the circle is counterclockwise, it is labeled S.

a. 

b. 

Switch H and CH₃

It looks like an S isomer, but we must reverse the answer, S to R.

R isomer
12. How is compound A related to compounds B–E? Choose from enantiomers, diastereomers, constitutional isomers, or identical molecules.

Recall that Enantiomers are compounds that are mirror images and are not superimposable. Another way to think of them is that they have complete opposite R and S designations. Diastereomers differ in at least one but not all stereocenters. They are also considered stereoisomers that are not mirror images of each other.