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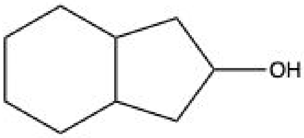
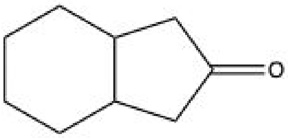
Chem 51A
Professor King
https://sites.uci.edu/ochemtutors/

Midterm 2 Review Worksheet

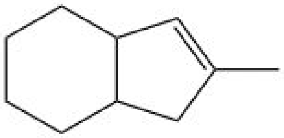
1. Rank the following compounds in order of increasing melting point.



A



B

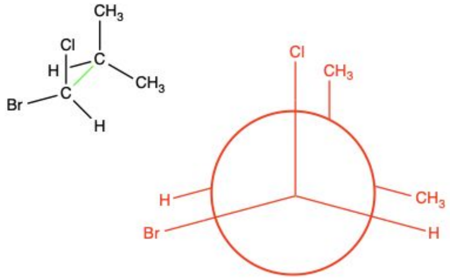


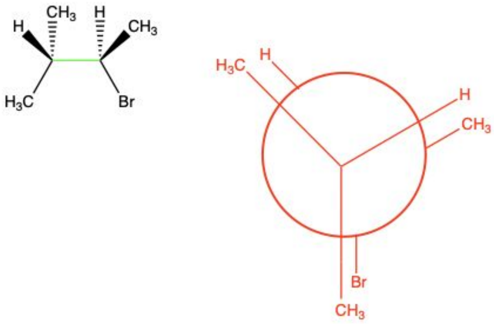
C

C<B<A ; C(VDW) < B (VDW, DD) < A (VDW,DD, H-Bonding)

An increase in strength of intermolecular forces corresponds to an increase in melting point.

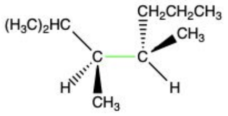
2. Convert each molecule to a Newman projection around the indicated bond.





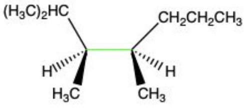
Tip: To draw a Newman projection, visualize the carbons as one being in the front and the other in the back. The C-C bond itself isn't drawn.

3. Classify each conformation as staggered or eclipsed around the indicated bond, and rank the conformations in order of increasing stability.



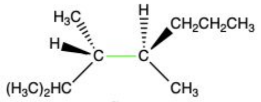
A

Staggered (isopropyl and propyl are gauche)



B

Eclipsed (2 largest groups are eclipsed —> highest energy —> least stable)



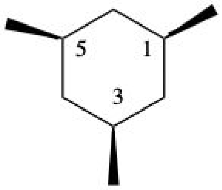
C

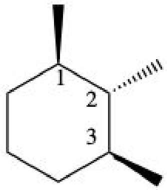
Eclipsed (second highest energy)

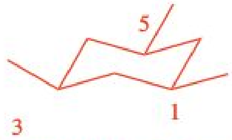
Increasing stability: B < C < A

Staggered conformations are at the energy minmia while eclipsed conformations are at the energy maxima. Higher energy —> less stable.

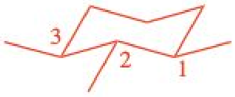
4. Draw the more stable chair conformation for each of the following trisubstituted cyclohexanes.







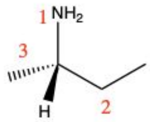
All equatorial methyl groups.



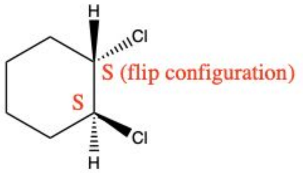
All equatorial methyl groups.

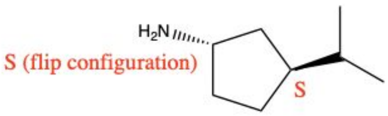
The more stable chair conformation is the one in which the larger alkyl group is in the more “roomy” equatorial position.

5. Label each stereogenic center as R or S.



S (H is not drawn back —> flip configuration)

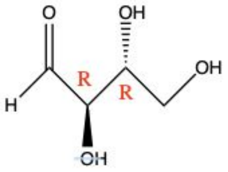




6. (S)-Lactic acid has a specific rotation of +3.8. If the ee of a solution of lactic acid is 60%, what is [α] for this solution?

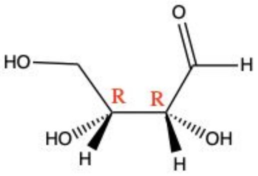
ee = (([α] mixture) / ([α] pure enantiomer)) x 100
0.6 = (([α] mixture) / 3.8) x 100
[α] mixture = **+ 2.3**

7. How is each compound related to the simple sugar D-erythrose? Is it an enantiomer, a diastereomer, or an identical molecule?



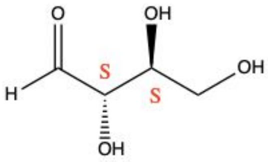
D-erythrose
2R, 3R

a.



2R, 3R —> identical

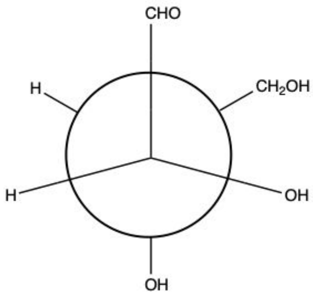
b.

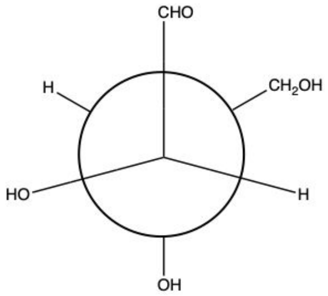


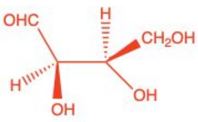
2S,3S —> enantiomer

Reminder: enantiomeric pairs have opposite configurations at each of the stereocenters.

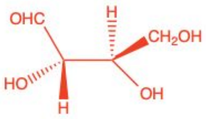
8. Looking at the Newman projections below, how are the compounds related (identical molecules, enantiomers, or diastereomers)?







R, R

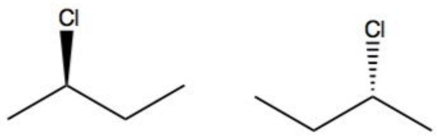


S, R

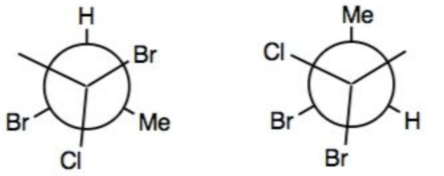
Diastereomers

Reminder: diastereomeric pairs have the same configuration at one of the two stereocenters and opposite configuration at the other.

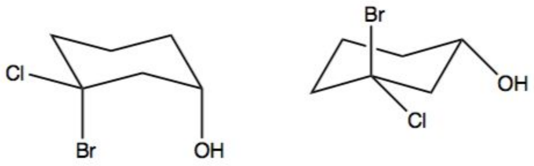
9. For each pair of structures, indicate whether they represent enantiomers, diastereomers, constitutional isomers, or identical compounds.



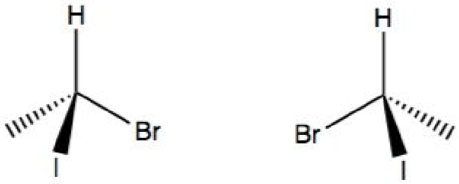
a. identical compounds



b. diastereomers

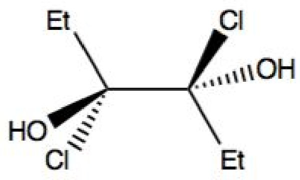


c. diastereomers

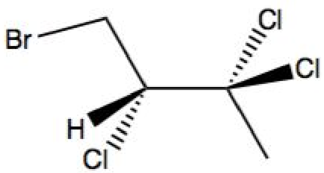


d. enantiomers

10. Explain why compound A has no enantiomer and compound B has no diastereomers.



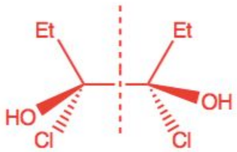
A



B

REMEMBER: Explanations should typically be limited to one sentence.

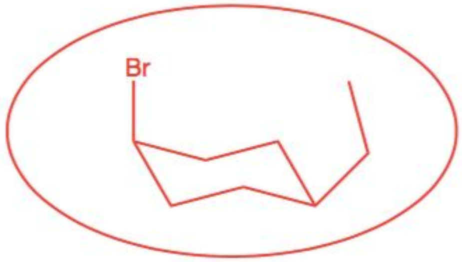
a. There are no enantiomers because the molecule has a plane of symmetry, so the mirror image will be superimposable.



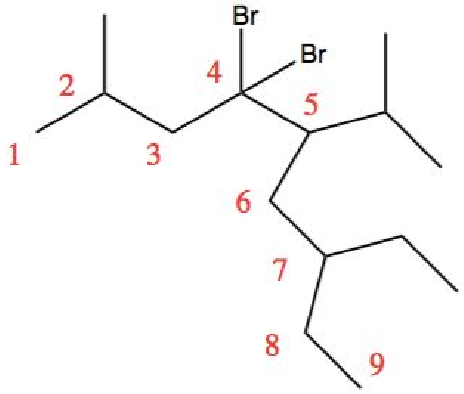
(remember that rotation about the sigma bond is possible)

b. Compound B has no diastereomers because there is only one stereoisomer.

11. Draw the two possible chair diagrams for *cis*-2-bromo-1-methylcyclohexane. Circle the most stable conformation.



12. Use IUPAC nomenclature to name the following compound.



4,4-dibromo-7-ethyl-5-isoproyl-2-methylnonane

Steps to naming:

1. Unbranched chains named according to number of carbons
2. If branched, find the **longest continuous chain → parent chain**
    a. If 2 or more chains of the same length, choose the one with more branches
3. Number the carbons of the parent chain from one end to the other in direction that gives 1st branch the lower number
4. Name each branch(substituent) and identify carbon number of parent chain it occurs at
    a. If 2 or more substituents at one carbon, use the number twice
    b. If 2 or more substituents are identical, use prefix **di-,tri-,tetra-,** etc
5. Name substituents first, then name the parent chain
    a. Put dashes between numbers and letters
    b. Substituents named in **alphabetical order** (only prefixes iso, neo & cyclo considered, ignore prefixes like di-or tert-)

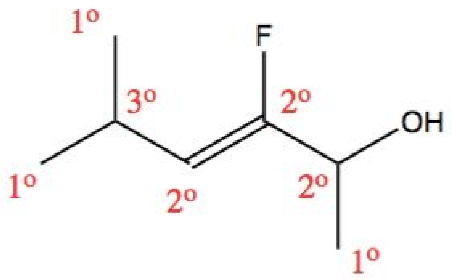
For this problem:

1. This compound is branched
2. The longest chain is 9 carbons → parent chain is nonane
3. Number starting from the top
    a. If started from the bottom, first substituent at the 3rd carbon
    b. If started from the top, first substituent at the 2nd carbon
4. Naming substituents
    a. 2-methyl (methyl at 2nd carbon)
    b. 4,4-dibromo (2 bromo substituents so use suffix di-, both at 4 so use the number 4 twice)
    c. 5-isopropyl (isopropyl group at 5th carbon)

    d. 7-ethyl (ethyl group at carbon 7)
5. Put it all together, substituents in alphabetical order
    a. 4,4-dibromo-7-ethyl-5-isoproyl-2-methylnonane

13. Why is/are ____ better than ____ ?
    a. Staggered, eclipsed
       Staggered conformations are more stable because eclipsed conformations have torsional strain
    b. Anti, gauche
       For anti conformations, the two largest groups are 180º from each other, while gauche conformations have , the two largest groups are 60º from each other. Thus, are more stable because gauche conformations have steric strain.

14. For the following molecule, label all the carbons as primary, secondary, tertiary, or quaternary.



primary carbon (1°) - bound to 1 other carbon
secondary (2°) - bound to 2 other carbon s
tertiary (3°) - bound to 3 other carbons
quaternary (4°) - bound to 4 other carbons

15. A specific drug has an enantiopure specific rotation of its (-) enantiomer of -45°.
    a. What is the observed rotation for a solution of the drug that contains 0.85 g of the (+) enantiomer and 0.12 g of the (-) enantiomer in 125 mL of the solvent?

       0.85 g-0.12 g= 0.73 g (+)
       +45°x0.85 g/125= **0.306**

b. What is the specific rotation of the positive enantiomer?

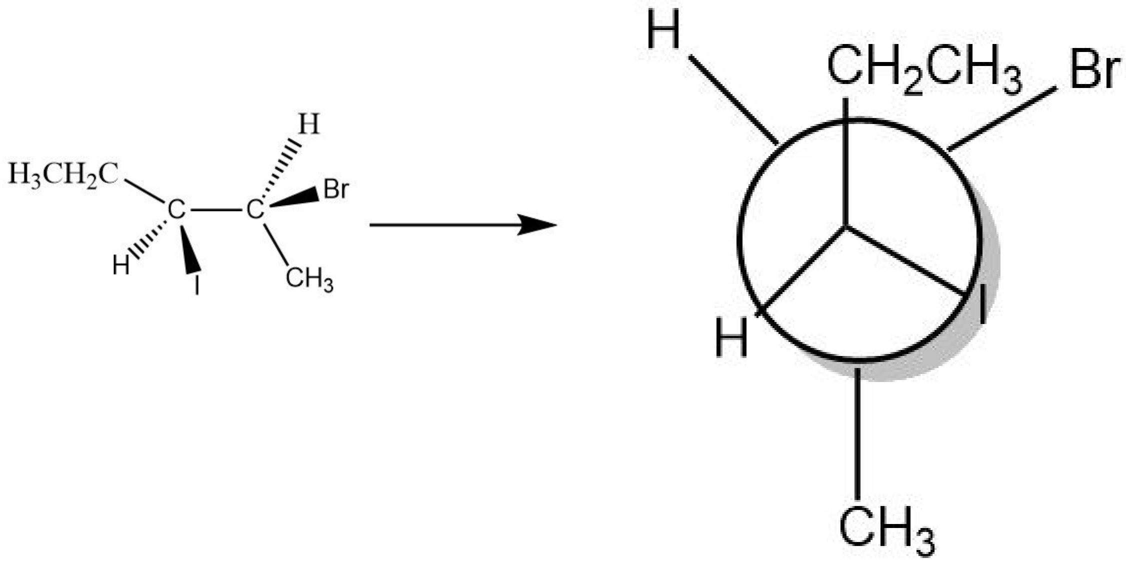
45°, since they are enantiomers, there will be a specific rotation of 0, meaning equal amounts of the positive enantiomer and equal amounts of the negative enantiomer.

c. Calculate the %ee of a solution with a specific rotation of -27°.

% ee= -27/-45 x 100%= **60.0% (+)**

16. For the following compound:

a. Assign R, S configurations for any stereocenters present
b. Draw the Newman projection of how the compound appears



Left stereocenter: S
Right stereocenter: R

17. For the following compounds below, answer the following questions

A) $CH_3CH_2CH_2OH$
B) $CH_3CH_2CH_2Br$
C) $CH_3CH_2CH_2F$
D) $CH_3CH_2CH_2NH_2$
E) $CH_3CH_2CH_2N(CH_3)_2$

a. Which compound(s) can form intramolecular hydrogen bonds? A, D
b. Which compound(s) can form hydrogen bonds with a solvent such as methanol? C, E
c. Which compound(s) cannot form hydrogen bonds at all? B

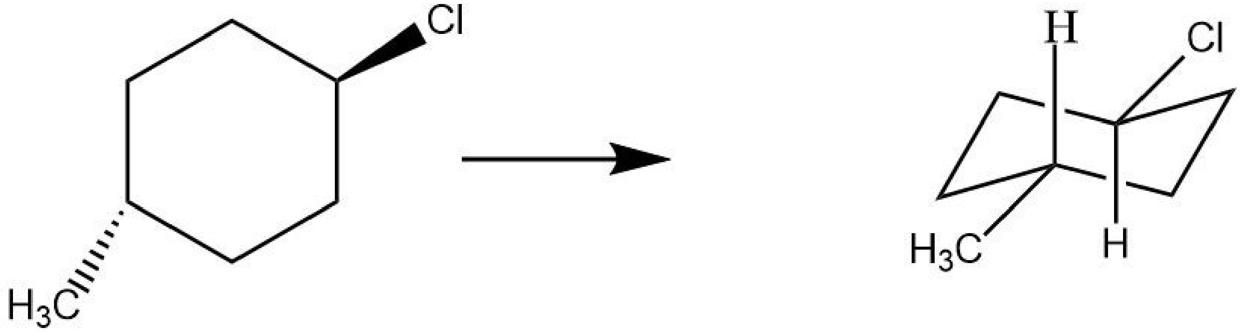
Memorization Tips:

18. The total number of _stereoisomers___________________________ will not exceed _2^n______, where n is

equal to the number of __tetrahedral stereocenters_______________________.

Enantiomers have _opposite configurations____________________________ at each stereocenter.

19. Draw the chair conformation for the following compound:



Key Tips for Chairs!!

- Axial bonds point in the SAME direction as the point of the chair that they are attached
- Equatorial bonds point SLIGHTLY UP @ the carbons that have axial bonds pointing DOWN and SLIGHTLY DOWN at carbons that have axial bonds pointing UP.

MESO Compounds: ONE of the stereoisomers has a plane of SYMMETRY!
A meso compound is ONLY possible when a molecule can be divided into structurally identical halves!

Remember the difference between conformation and configuration.

- Confirmation: Rotation about the sigma is possible without bond breakage
- Configuration: Rotation not possible, have to break and form bonds

TIP: Be comfortable with converting between Newman projection and skeletal structure and between chair conformation and cyclohexane

GOOD LUCK!!