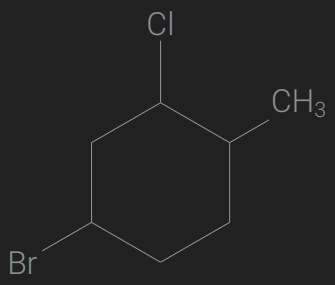
Contents

Week 6

Monday, November 2

1. What is the name of the following molecule?



   - ▷ **4-bromo-1-chloro-2-metyhlcyclohexane**
     - Lowest sum and alphabetically ordered.

2. What is the definition of a molecular conformation?

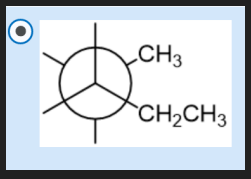
   - ▷ **A geometric arrangement in space of a molecule that has a low energy pathway to rearrangement**
     - **Conformations**: the variety of possible three-dimensional shapes of a molecule that are interchangeable by low energy pathways.
       - Conformations vary in potential energy.
       - Changes due to rotation about σ bonds.

3. What is the following molecule?

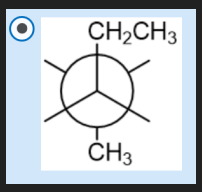
   (The package that draws newman projections is not compatable with the font I use... working on a fix, but can't draw them at the moment)

   - ▷ **pentane**
     - Front portion has 3 carbons in the chain: CH_3 (1), CH_2 (2), and the 4° carbon (3) in the center.
     - The circle represents the σ bond between the carbon behind it, so thats (4).
     - The methyl (CH_3) on the back portion is (5).

4. For the molecule in the previous question, which conformer is the gauche form of the molecule?
    - ▷ **choice 1**
    - ▷ Can't draw newman projections currently; it's broken... but here's this lame screenshot:



        - **Gauche interaction**: unfavorable intereaction between groups, causing an increases in energy due to electron cloud repulsion.
        - Gauche intereaction is a type of steric intereactions present at $\approx \pm 60°$ the next eclipsed conformation.
5. For the same molecule, which conformation corresponds to the most stable form?
    - ▷ **pick number 1 m'lord**
    - ▷ ugggghhhhhhhhhhhhhh so ugly :(



        - Other forms represent an eclipsed form and the gauche interaction, both which increases potential energy due to increased torsional strain.
        - More notes for reference:
            - **dihedral (torsional) angle**: the angle between substituents of front and back carbons as the σ bonds rotates.
            - **Staggered conformation**: lowest energy conformation, when two substituents are at maximum dihedral angle from each other.
            - **Eclipsed conformation**: the highest energy conformation, when two substituents are at the minimum dihedral angle from each other.

6. For which molecule will the energy of conversion (E_{act}) be the greatest?
   - ▷ **butane**
     - I don't really know what E_{act} is, but I assume it's the energy required to go through the interchangeable pathway.
     - Costs of butane:
       - $19\,kJ/mol$ (eclipsed with methyl overlap; once)
       - $16\,kJ/mol$ (eclipsed, no methyl, but with gauche; twice)
       - $3.8\,kJ/mol$ (gauche only; twice)
     - I'm not sure if you add them up or just take max, but either way butane has the greatest out of ethane, propane, and methane.
7. Why is the cyclohexane ring more stable than rings of other sizes?
   - ▷ the bond angles are all nearly $109.5°$
   - ▷ the ring strain is at a minimum
   - ▷ the overlap of the sp^3 hybrid orbitals is at a maximum
   - ▷ **all of the above**
     - This is true in the most stable, chair conformaions at least.
8. Why can't the cyclobutane ring be square planar?
   - ▷ **the 2s orbitals wouldn't overlap well** OR the sp^3 orbitals wouldn't overlap well
     - Cyclobutane adopts a slightly puckered conformation in order to reduce angle strain (and eclipsed H)... which I now assume is the because 2s orbitals after getting the question wrong twice.
9. In the cartoon picture shown below, who's on the chair and who's on the boat forms of cyclohexane?
   - ▷ **she's on the chair and he's on the boat**
     - Hmmmmmmmmmmm....
10. What is the total energy for the cyclohexane ring flipping process?
    - ▷ **12.1**
      - Appears to be just the cost of the first flip to the half chair.
      - Can't seem to find good explanation to why, however.