Activity 3

Understanding Conformational Analysis

Model 1: Understanding Model Kits

The Pieces:

White spheres = Hydrogen atoms
Red spheres = Oxygen atoms
Blue spheres = Nitrogen atoms
Green spheres = Halogens

Bent sticks = bonds (black = sp³ bonds to carbon atoms; red = sp³ bonds to oxygen atoms)
*the bend represents a carbon atom.

Tasks:

1. Figure out how to construct a model of methane (CH₄). Remember that only the technician may assemble the model with suggestions from the other team members.

2. Next assemble a model of ethane. Use spheres to represent hydrogen atoms and ensure that each member of the team can clearly identify the carbon atoms.

Model 2: Conformations of Ethane

In your model of ethane, designate one carbon atom as C1 and the second as C2. Now rotate the about the carbon-carbon single bond. As you rotate around the C1-C2 bond, look down this bond.

Critical Thinking Questions:

1. As a group discuss and describe what you see looking down the C1-C2 bond as you rotate the back carbon? Describe your observations in complete sentences.
2. How many different orientations, or conformations, of hydrogen atoms are possible between C1 and C2? Explain.

3. In which conformation would you consider the hydrogen atoms from C1 to be *eclipsed* with those of C2? Please describe using a complete sentence. **Hint:** Think about what happens during a solar or lunar *eclipse*.

4. In which conformation would you consider the hydrogen atoms from C1 to be *staggered* with those of C2? Explain.

---

**Model 3: Newman Projections**

Newman Projections are structural formulas on paper that we use to relate conformations that we see in three dimensions. The model below shows the Newman Projections for both conformations of ethane.
Critical Thinking Questions:

5. Study the Newman projections shown above for ethane. What does the point denoted by the arrow signify (CTQ 5)?

6. What does the circle denoted by the arrow signify (CTQ 6)?

7. How do you determine which hydrogen atoms are attached to either C1 or C2? Explain in detail.


a. Are any of these conformations the same? Are any different? Explain why.
b. An *anti* conformation occurs when any substituent group is at the position furthest away from another substituent (180° apart – the *dihedral* angle). With this information, which staggered conformation(s) would be considered *anti*?

c. Another staggered conformation is the *gauche* conformation. This occurs when the angle between the two substituents on C2 and C3 is 60° apart (the *dihedral* angle). Which Newman Projection(s) represents *gauche* conformations?

9. Draw three eclipsed conformations for butane again looking down the C2-C3 bond. Are any of these conformations the same? Are any different? Explain why.
Model 4: Conformational Stability

We know that molecules adopt certain shapes, or geometries, as a way of trying to minimize the repulsion between those bonding and nonbonding electrons. In doing so, we say that molecules achieve a state of minimum energy and maximum stability. This same idea can be applied to the different conformations of ethane. The energy diagram below illustrates this idea.

Critical Thinking Questions:

10. Looking at the two conformations for ethane, why is the staggered conformation lower in energy (i.e. more stable) than the eclipsed conformation? Explain.
11. Using your model for butane, what conformation(s) of butane would be the most stable and why?

12. What conformation(s) of butane would be the least stable and why?

13. Complete the energy diagram shown below for butane by drawing the appropriate Newman Projections in the boxes below.