

4.1: Conformation Analysis of Alkanes

4.1.1 Conformation

At a molecular level, a property of σ (sigma) bonds in alkane is that the bonds keep on rotating. For the example of ethane (CH_3CH_3), one methyl (CH_3) group is able to rotate around the C-C bond freely without any obstacles.

It is highly recommended that the molecular model is used here to “see” the bond rotation. With a molecular model on hand, you can hold one methyl group steady, and rotate the other methyl group.

The C-C bond is formed by the $\text{sp}^3\text{-sp}^3$ orbitals overlapping and the bond is cylindrically symmetrical, so rotation about the bond can occur easily and the molecule does not seem to change. However, a closer look indicates that the rotation of the C-C bond **does** result in a different spatial arrangement of hydrogen atoms in the molecule, as shown below:

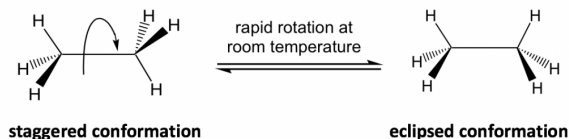


Figure 4.1a Two conformers of ethane in perspective formulas

The different spatial arrangements of the atoms/groups that result from the single bond rotation are called **conformations**. Molecules with different conformations are called **conformational isomers** or **conformers**. The two extreme conformations of ethane coming from the C-C rotation shown above are: the **staggered conformation** with all of the H atoms spread out, and the **eclipsed conformation** with all of the H atoms overlapped.

In the study of conformation, it is convenient to use certain types of structural formulas. The formula used in the drawing above is the **perspective formula** (see section 2.1.1) that shows the side-view of the molecule. In perspective formulas, solid and dashed wedges are used to show the spatial arrangement of atoms (or groups) around the sp^3 carbons.

Another structural formula is the **sawhorse formula** that shows the tilted top-view of the molecule.

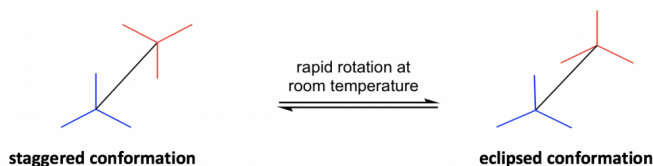


Figure 4.1b Two conformers of ethane in sawhorse formulas

The most commonly applied formula in conformation analysis is the **Newman projection** formula.

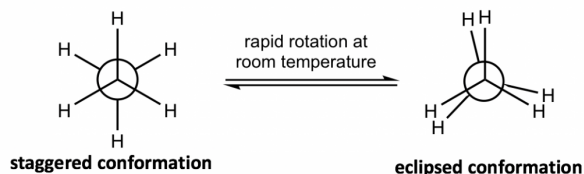


Figure 4.1c Two conformers of ethane in Newman projections

How to draw a Newman projection

To draw a **Newman projection**, we will imagine **viewing** the molecule *from one carbon to the next carbon atom directly along a selected C-C bond*, as shown below, and follow the rules:

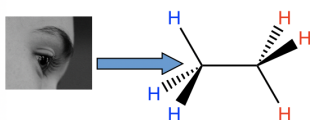
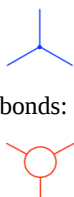


Figure 4.1d Viewing of the molecule

- The front carbon atom is shown as a point with three other bonds:

- The rear carbon atom is shown as a circle with three other bonds:



- Put the two carbons together to get the Newman projection of the staggered conformation:



- From the staggered conformation, fix the front carbon in place, and rotate the rear carbon by 60° to get the eclipsed conformation:



Note: In eclipsed conformers, the C-H bonds are supposed to be completely overlapped; however, to make the *rear* groups still visible, the bonds on the rear carbon are intentionally drawn slightly tilted.

4.1.2 Conformation Analysis of Ethane

Next, we will do a conformation analysis of ethane by using the Newman projections. A **conformation analysis** is an investigation of energy differences and relative stabilities of the different conformations of a compound.

The two conformations of ethane, staggered and eclipsed, are different and therefore should be in different energy levels. You may also predict intuitively that the staggered conformation is more stable and is lower energy, because the C-H bonds are arranged as far apart as possible in that conformation. That is correct! In eclipsed conformations, the H atoms on the front carbon are overlapping with the H atoms on the rear carbon, and this arrangement causes the repulsion between the electrons of C-H bonds of the two carbons. This type of repulsion is called the **torsional strain**, also known as the eclipsing strain. Due to the torsional strain, the eclipsed conformer is in the energy level that is 12 kJ/mol (or about 2.9 kcal/mol) higher than the staggered one. This can be represented graphically in a potential energy diagram as shown in Figure 4.1f.

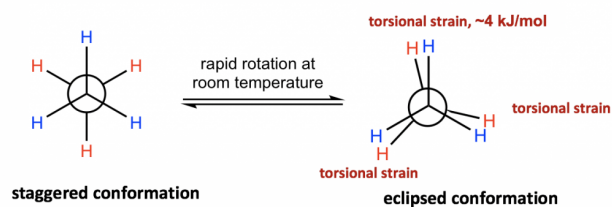


Figure 4.1e Staggered vs. eclipsed conformation

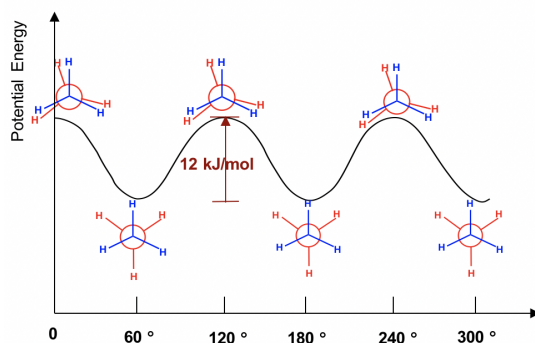


Fig. 4.1f Potential Energy of Ethane vs the Angle of Rotation about the C-C bond

Because of this energy difference, an energy barrier must be overcome when the rotation about the C-C bond occurs. However, this energy difference in ethane is rather small, and the kinetic energy of molecules at room temperature is high enough to cover it. So at room temperature, the changes from staggered to eclipsed conformers occur millions of times per second. Because of these continuous interconversions, these two conformers cannot be separated from each other. However, at any given moment, about 99% of the ethane molecules will be in a staggered conformation because of their higher stability.

4.1.3 Conformation Analysis of Propane

A similar analysis can be applied to propane as well. We will find that there are still two types of conformations, staggered and eclipsed, resulting from the rotation. The difference between propane and ethane is that there is a methyl (CH_3) group connected on the rear carbon for propane. However, that does not affect the relative stability, and the staggered conformer is more stable and in lower energy.

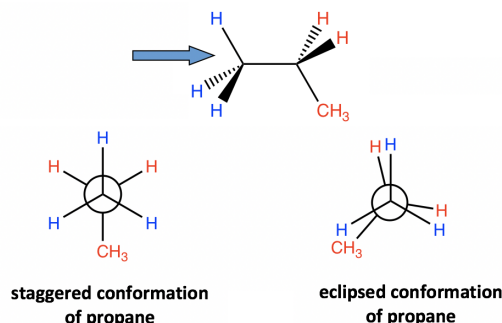


Figure 4.1g Staggered and eclipsed conformation of propane

4.1.4 Conformation Analysis of Butane

There are three C-C bonds in butane, and rotation can occur about each of them. If we pick up C1-C2 (or C3-C4) for the study, the situation is almost the same as propane, with the ethyl CH_2CH_3 group replace the CH_3 group. However, if we consider the rotation about the C2-C3 bond, the situation will be much more complex.

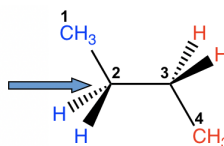


Figure 4.1h Conformation analysis of butane by viewing along C2-C3 bond

For both carbon atoms, C2 and C3, there are two hydrogen atoms and one methyl CH_3 group bonded with. We can start with the conformer in which the two CH_3 groups are **opposite** to each other, then fix the front carbon and do 60° rotations of the rear carbon to investigate **all** the possible conformations.

Exercises 4.1: Draw all the possible conformers of butane from viewing along the C2-C3 bond. Finish this practice by yourself before continue reading!

Tips for drawing all the possible conformers about a certain C-C bond:

- View along that C-C bond; circle and decide what atoms/groups are connected on each carbon;
- Start with the staggered conformation in which the largest groups on each carbon are opposite (far away) to each other (this is called the “*anti*” conformation as we will learn later);
- Keep the groups on one carbon “fixed”, and rotate the groups on the other carbon at 60° angles. Repeat the rotation five times, and you should get total of six conformers.

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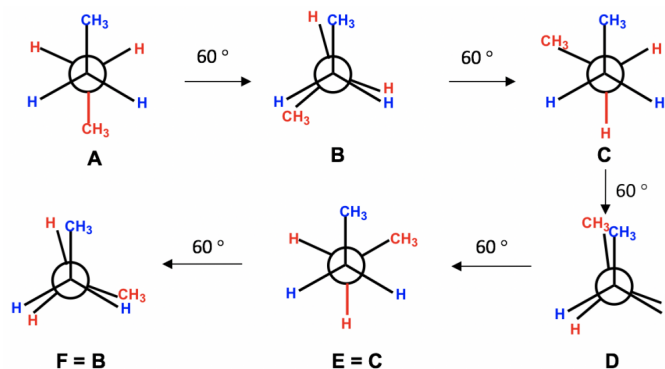


Figure 4.1i All the conformers of butane by viewing along C2-C3 bond

Among all the six conformers obtained, there are three staggered and three eclipsed. Staggered conformations **C** and **E** should be in the same energy level because the groups are arranged in equivalent way between these two conformers. Similarly, eclipsed conformations **F** and **B** are also in the same energy level. So our studies can be focused on the four conformers, **A**, **B**, **C** and **D**, that are different in terms of energy and stability.

Between the two staggered conformers **A** and **C**, **A** is more stable than **C** because the two methyl CH_3 groups in **A** are as far apart as possible. This most stable staggered conformation is called the **anti** conformation (*anti* is Greek for “opposite”). In **anti** conformations, the largest groups on the front and rear carbon are 180° opposite to each other. The other staggered conformation **C** is called a **gauche** conformation, in which the two large groups are adjacent and are 60° to each other. With the large groups being close to each other in gauche conformers, the molecule experiences **steric strain**. **Steric strain** is the strain that is caused when atoms (or groups) are close enough together that their electron clouds repel each other. Steric strain only matters when the groups are close to each other (less or equal to 60°), so steric strain does not apply in anti conformations. The magnitude of steric strain also depends on the size of group; the larger the size, the higher the steric strain. As a result, there is no steric strain between two small hydrogen atoms, even if they are close to each other.

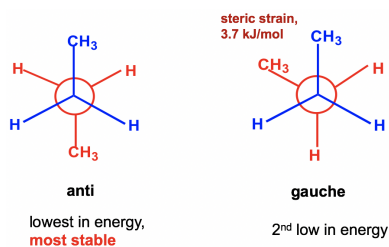


Figure 4.1j Anti and gauche conformations

Between the two eclipsed conformers **B** and **D**, **D** is less stable than **B**, because the two CH_3 groups are eclipsing (overlapping) each other in **D**, causing both torsional and steric strains.

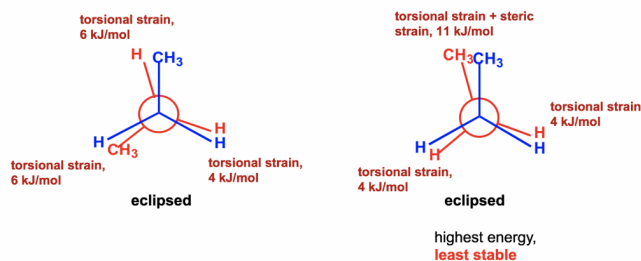


Figure 4.1k Comparison between the two eclipsed conformations

The energy difference of all the conformers obtained from the rotation about the C2-C3 bond are shown in the potential energy diagram **Fig. 4.1l**. The curve is more complex than that of ethane since there are four different energy levels corresponding to four conformers with different stabilities. Even the energy barriers for the rotations are larger than that of ethane, but they are still not high enough to stop rotation at room temperature.

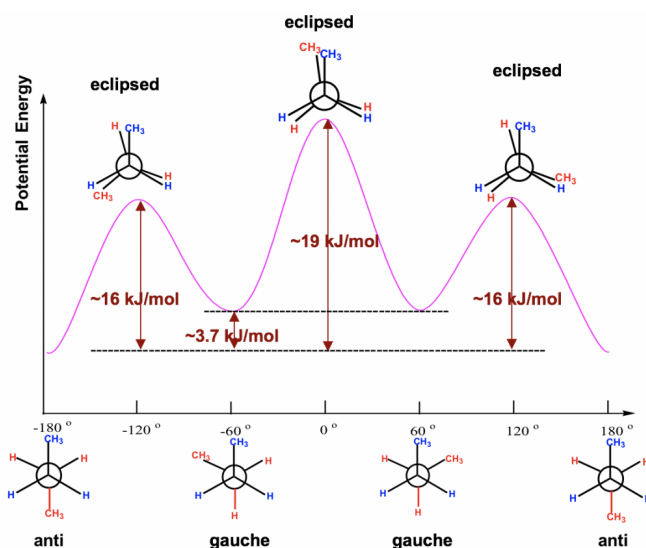


Figure 4.11 Potential Energy of Butane vs the Angle of Rotation about the C2-C3 bond

Exercises 4.2

Draw all conformers for 3-methylpentane by viewing along the C2-C3 bond, and order them from the most stable to least stable.

[Answers to Practice Questions Chapter 4](#)

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