Conformational analysis of 3-methylpentane

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1. Introduction

Conformational analysis is the study of the different orientation of atoms of a molecule in space that a molecule can adopt due to rotation across a carbon – carbon bond. It's particularly important in organic chemistry, where molecules often contain single bonds around which atoms or groups of atoms can rotate. Understanding the different conformations and their associated energies helps chemists predict the stability and reactivity of molecules.

1.1. Conformational analysis:

1.1.2 What is Conformational Analysis?

- Conformations are different spatial arrangements of a molecule that can be converted into one another by rotation around single bonds without breaking any covalent bonds.
- The flexibility to adopt different conformations is due to the ability of single bonds to rotate. Double and triple bonds are more rigid and do not allow such freedom of movement.

1.1.3 Why is Conformational Analysis Important?

- **Chemical Properties**: Different conformations can have different reactivities, and stabilities. The most stable conformation is often the one with the lowest energy.
- **Biological Relevance**: In biomolecules like proteins and DNA, conformations play a critical role in their function and interaction with other molecules.
- **Pharmaceuticals**: Understanding the preferred conformations of a drug molecule can be useful in its design and how it interacts with biological targets.

1.1.4 Applications of Conformational Analysis

- **Chemical Synthesis**: Understanding conformations helps chemists design synthetic routes and predict reaction outcomes.
- **Drug Design**: Identifying the preferred conformation of a drug molecule can impact its efficacy and safety.

- **Biological Studies**: Conformational changes in proteins and other biomolecules are key to their function in biological processes.

2. Process of Conformational analysis:

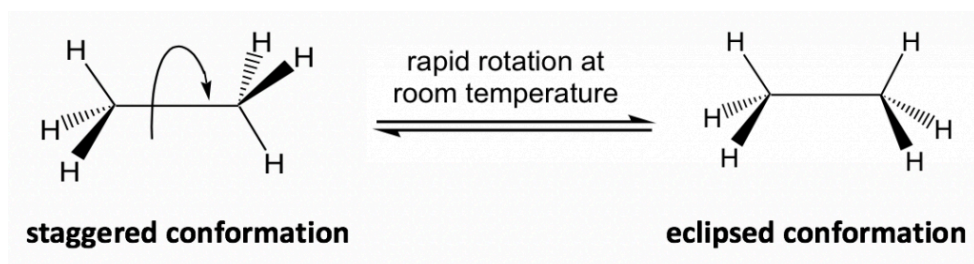### 2.1 Tools for Conformational Analysis

- **Newman Projections**: A way to visualize the conformations of a molecule by looking along a specific bond.
- **Sawhorse Projections**: A tilted view of a molecule to show its conformation.
- **Molecular Modelling Software**: Computer programs that allow you to visualize and analyse different conformations. We are using Jmol in this report.

2.2 Common Concepts in Conformational Analysis:

- **Eclipsed and Staggered Conformations**: In simple molecules like ethane, rotation leads to different conformations. The eclipsed conformation has higher energy due to torsional strain, while the staggered conformation is more stable.

2.3 Procedure:

- The C-C bond is formed by the sp^3-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:
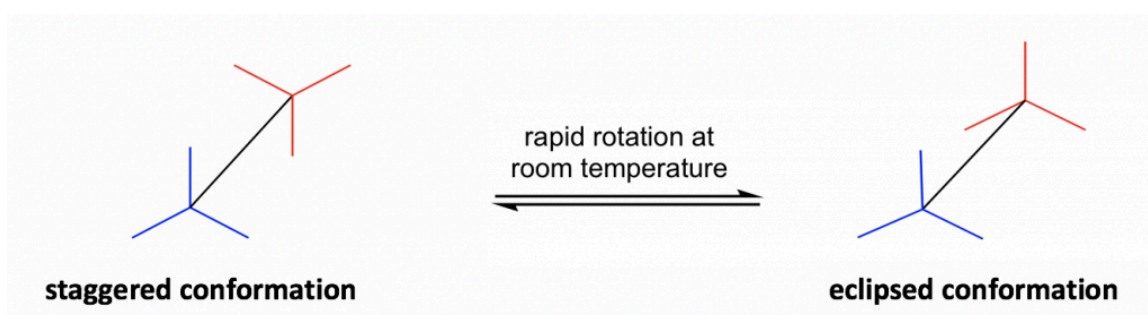

Two conformers of ethane in perspective formulas

- 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
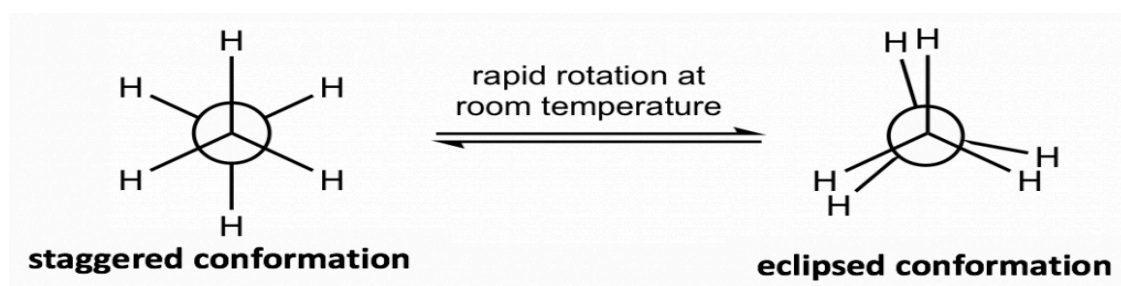
all of the H atoms spread out and the *eclipsed conformation* with all of the H atoms overlapped.

- 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** 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** which shows the tilted top-view of the molecule.

Two conformers of ethane in sawhorse formulas

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

Two conformers of ethane in Newman projections

- 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:

Viewing of the molecule

- The front carbon atom is shown as a point with three other bonds(C1)

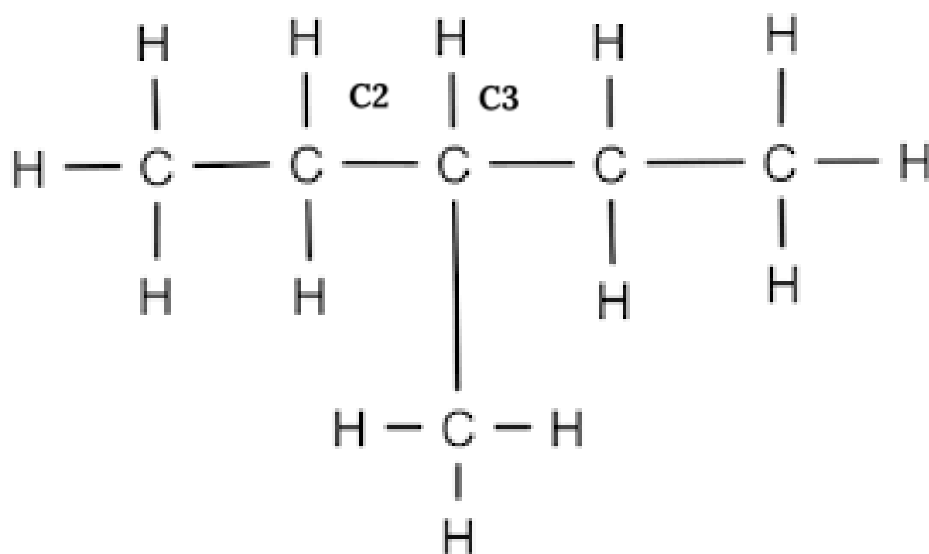- The rear carbon atom is shown as a circle with three other bonds(C2)

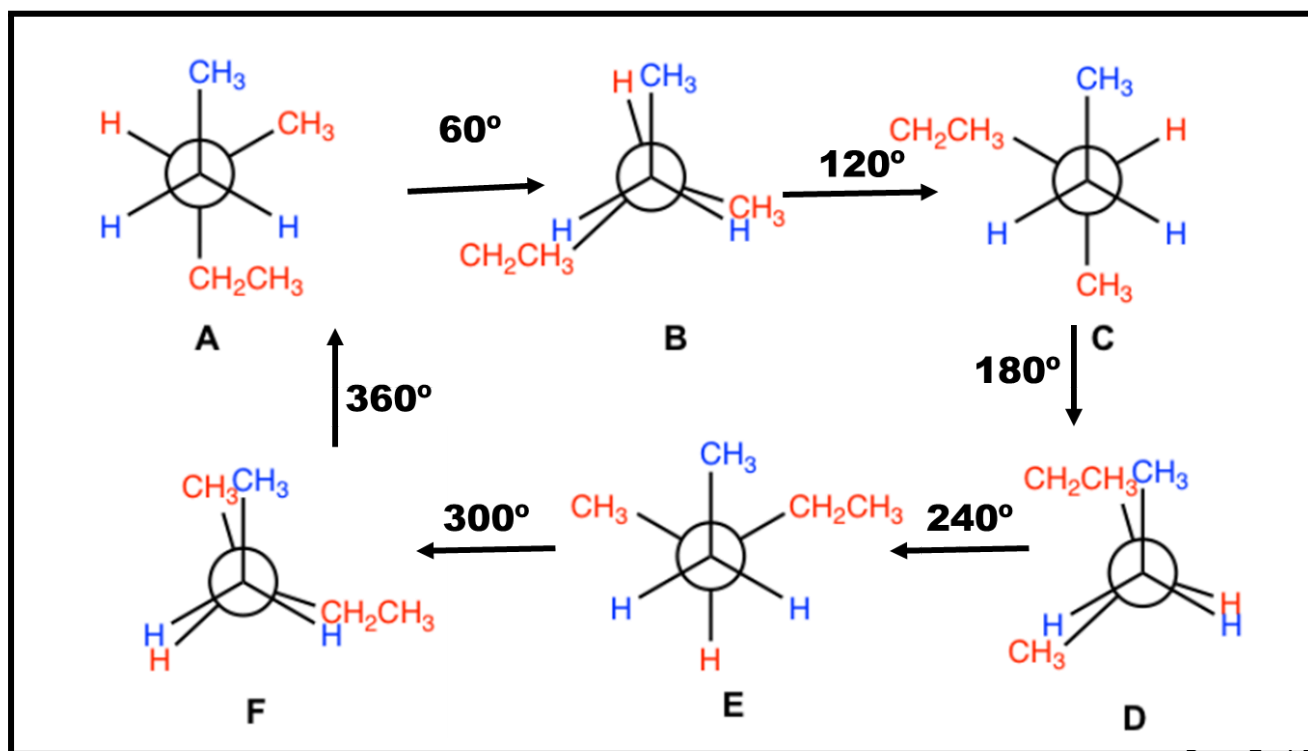- Put the two carbons together to get the Newman projection of the staggered conformation:

- From the staggered conformation, fix the front carbon in place and rotate the rear carbon by 60° to get the eclipsed conformation:
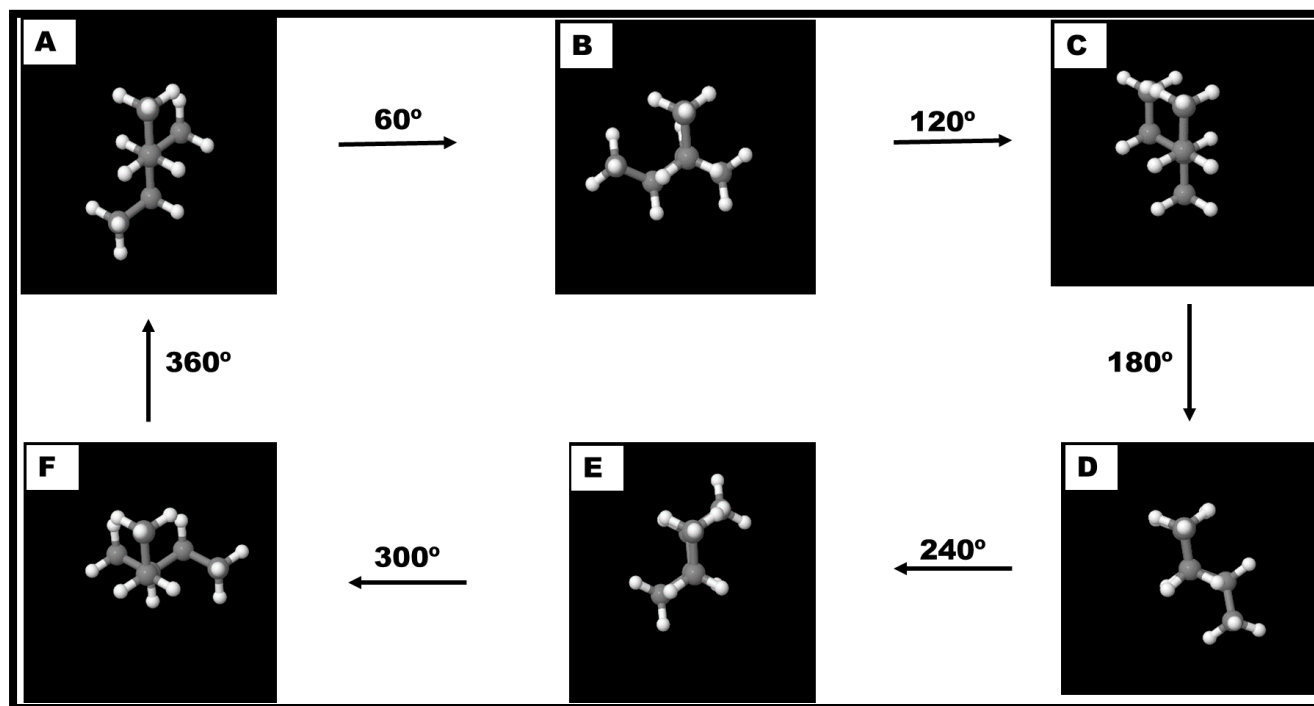
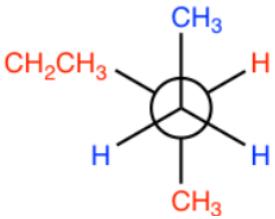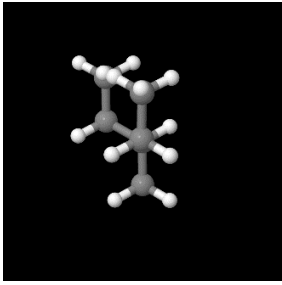## 3. Conformations of 3-methylpentane:

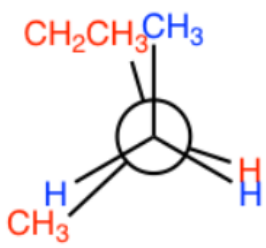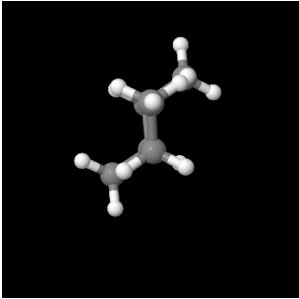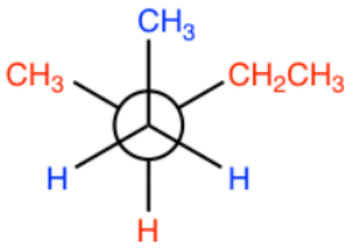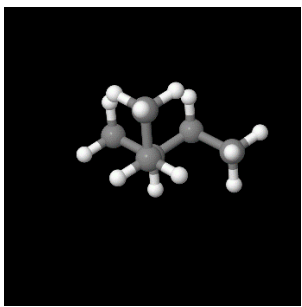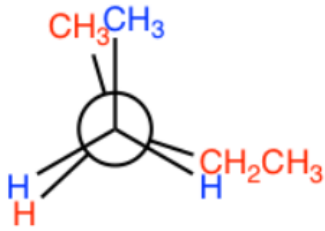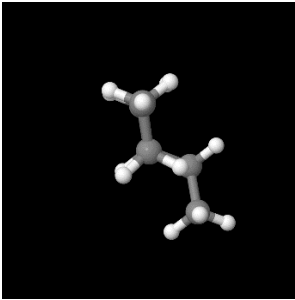## 3.1 2D diagram of conformations of 3-methylpentane

3.2 3D models of conformations of 3-methylpentane created using Jmol

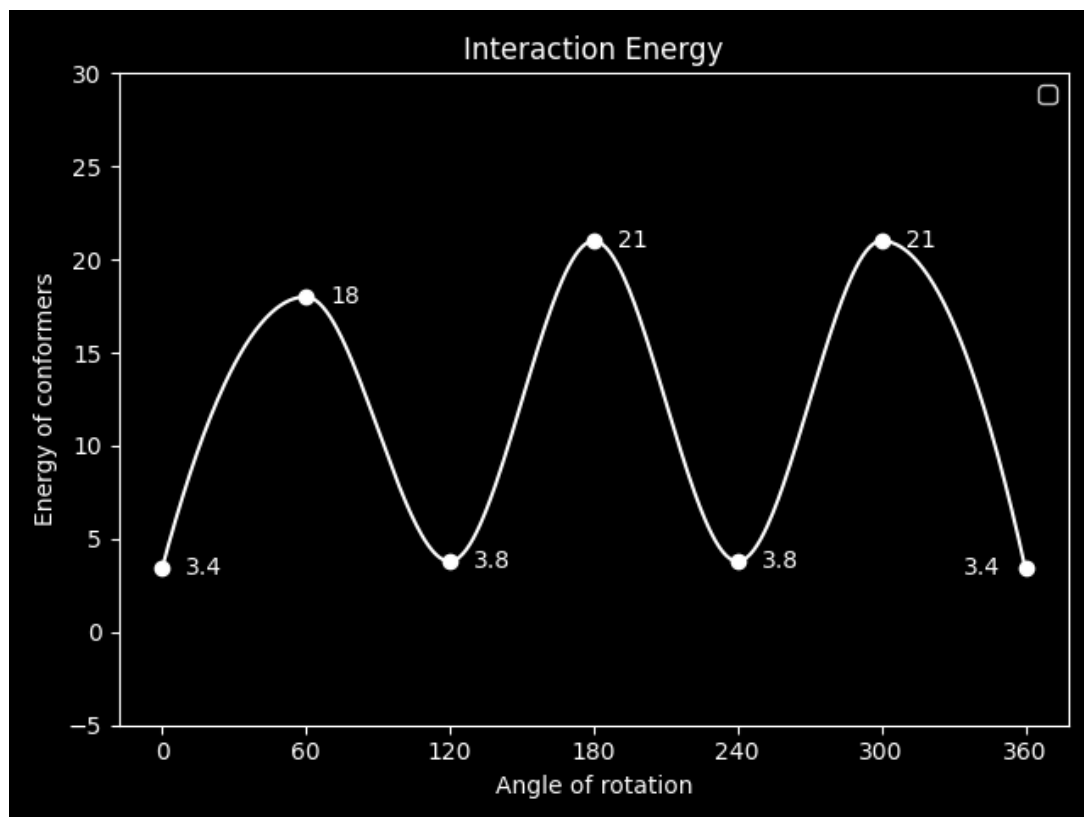## 3.3 Collective details of various conformers and their energies

2D picture	3D picture	Type of conformation	Energy
CH₃ H — CH₃ H — H CH₂CH₃ A		Staggered	3.4 kJ/mol
H CH₃ CH₃ H CH₂CH₃ B		Eclipsed	18 kJ/mol

 C		Staggered	3.8 kJ/mol
 D		Eclipsed	21 kJ/mol
 E		Staggered	3.8 kJ/mol
 F		Eclipsed	21 kJ/mol

3.4 Energy graph for conformations of 3-methylpentane

3.5 Results

- Number of conformers = 6
- Types of conformers = 2
- Eclipsed = 3
- Staggered = 3

4. Conclusion

- Staggered conformation of 3-methylpentane is the most stable, while eclipsed conformation is least stable
- The order of stability is given as,

A > C, E > B > F, D

Most stable   **least stable**

Creating the 3D model:

Drawing the 3D structure of 3-methylpentane molecule in Jmol interface

- Open Jmol interface select the model kit menu
- Select the carbon atom from the model kit.
- Click in the workspace to place a carbon atom. It will appear as a methane molecule
- Click on one of the hydrogen atoms to replace it with another carbon atom, extending the chain.
- Repeat this process until you have a five-carbon chain (pentane).
- Select another carbon atom from the model kit.
- Click on the third carbon atom of the pentane chain to attach this new carbon, forming 3-methylpentane.

Energy minimization of 3-methylpentane in Jmol interface

- Exit from the model kit menu
- Now right click on the molecule
- Select the energy minimization
- Rotate the conformer using model kit men

Save the 3D structure as .mol file

- Click the model kit menu
- In the drop-down list select the last option
- Click on the save file option
- Now the structure is saved in the .mol format