# 4.5: CONFORMATIONS OF HIGHER ALKANES

**Learning Objective**

- interpret and draw the rotation about a carbon-carbon single bond using Newman projections and sawhorse structures
- correlate energies of conformations with rotational energy diagrams and predict the most stable conformations for higher alkanes

## Pentane and Higher Alkanes

Pentane and higher alkanes have conformational preferences similar to ethane and butane. Each dihedral angle tries to adopt a staggered conformation and each internal C-C bond attempts to take on an anti conformation to minimize the potential energy of the molecule. The most stable conformation of any unbranched alkane follows these rules to take on zigzag shapes:

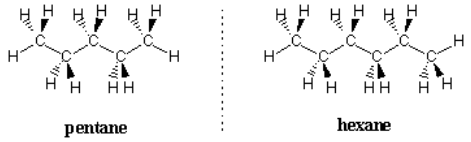



Figure %: The zigzag shapes of unbranched alkanes in their most stable conformations.

Let's analyze the staggered conformations of pentane in more detail, considering conformations about the $C_2 –C_3 $ and $C_3 –C_4 $ bonds. shows a few possible permutations. The most stable conformation is anti at both bonds, whereas less stable conformations contain gauche interactions. One gauche-gauche conformer is particularly unfavorable because methyl groups are aligned with parallel bonds in close proximity. This conformation is called syn. This type of steric hindrance across five atoms is called a syn-pentane interaction. Syn-pentane interactions have an energetic cost of about 3.6 kcal/mol relative to the anti-anti conformation and are therefore disfavored.

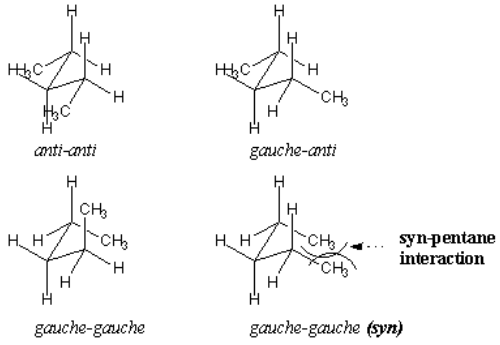
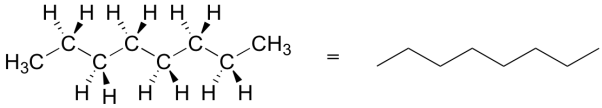


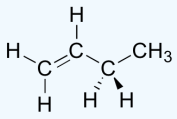

Figure %: Staggered conformations of pentane.



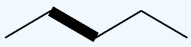
octane

**Exercises**

1. Draw Newman projections of the eclipsed and staggered conformations of propane.
2. Draw a Newman projection, looking down the $C_2$-$C_3$ bond, of 1-butene in the conformation shown below.

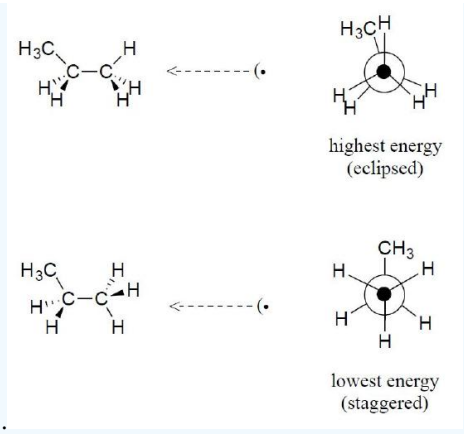


3. Draw the energy diagram for the rotation of the bond highlighted in pentane.



**Answer**

**1.**

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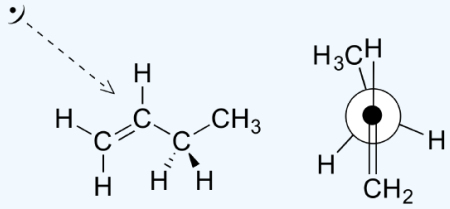
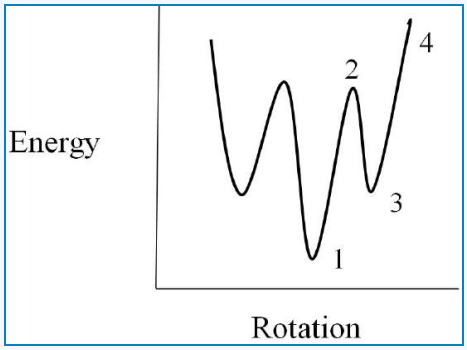
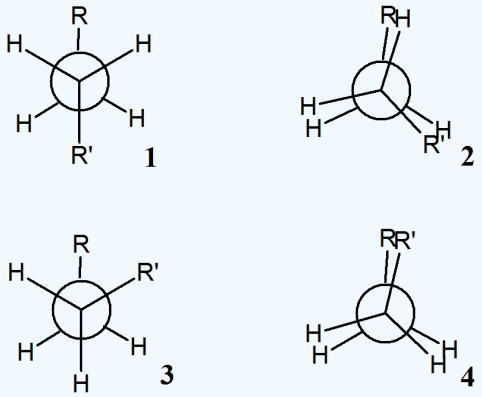


3.




R=Methyl
R'=Ethyl

## CONTRIBUTORS AND ATTRIBUTIONS

- Dr. Dietmar Kennepohl FCIC (Professor of Chemistry, Athabasca University)
- Prof. Steven Farmer (Sonoma State University)
- Organic Chemistry With a Biological Emphasis by Tim Soderberg (University of Minnesota, Morris)
- Jim Clark (Chemguide.co.uk)

- William Reusch, Professor Emeritus (Michigan State U.), Virtual Textbook of Organic Chemistry