An understanding of the factors that go into determining the lowest energy conformation of acyclic molecules is required to understand the stereochemical outcomes of many reactions. Here we will discuss how steric, electronic, and stereoelectronic effects influence the conformation of acyclic organic molecules.

**Ethane and Propane**

<table>
<thead>
<tr>
<th>Eclipsed Interaction</th>
<th>Energy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H-H} )</td>
<td>1.0</td>
</tr>
<tr>
<td>( \text{H-CH}_3 )</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Using the eclipsing interactions extracted from ethane and propane we can estimate all but one of the eclipsed butane conformations.

<table>
<thead>
<tr>
<th>Eclipsed atoms</th>
<th>( \delta E ) (kcal mol(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (H( \leftrightarrow )H)</td>
<td>+1.0 kcal mol(^{-1})</td>
</tr>
<tr>
<td>2 (H( \leftrightarrow )Me)</td>
<td>+2.8 kcal mol(^{-1})</td>
</tr>
</tbody>
</table>

\( \Delta E \) est = 3.8 kcal mol\(^{-1}\)

The value of +3.8 kcal/mol agrees quite well with the value of +3.6 reported by Allinger (*J. Comp. Chem.*, 1980, 1, 181-184.) His results are graphed below.
From Allinger's results we can determine the energetic value of eclipsing methyl groups:

\[
\Delta E = +5.1 \text{ kcal mol}^{-1}
\]

Thus we can see that the interaction between eclipsing methyl groups is worth 3.1 kcal/mol.

---

**Pentane**

**Allylic Strain**

The allylic stereocenter (marked with "***") and its substituents play an important part in determining the stereochemical outcome of reactions with the neighboring pi-bond. Allylic-1,3 and allylic-1,2 interactions (defined below) greatly affect the diastereoselectivity of reactions.

More can be read about A(1,3) strain here: *Chem. Rev.*, 1989, 89, 1841-1860.
Propene and 1-Butene

To understand the origins of A(1,2) and A(1,3) strain, we have to look at the consequences of introducing sp\(^2\) hybridized centers into our structures. The first major difference is the bond angle change from 109° to 120°.

Changing from propane to propene has major affects on the preferred conformation of the molecule. Propene now prefers to sit in an eclipsed conformation.

We can understand this change in preference by looking at the new orbital interactions that arise from the p-orbitals forming a pi-bond. New stabilizing and destabilizing interactions account for the stabilization of the eclipsed conformation and the destabilization of the staggered conformation, respectively.

Relevant Orbital Interactions:


These effects become more pronounced as we move to butane and 1-butene. The eclipsed methyl-methyl conformation is now lower in energy than the staggered conformation; however, it is not the lowest energy conformation.
Analysis of the torsional energy profile shows that the lowest energy conformation for 1-butene arises when one of the hydrogen atoms is in the plane of the alkene. We often times will refer to drawing these lowest energy conformations as the "H-in plane conformation."

2-pentene

Contributors

- Michael Di Maso (UC Davis)
- Jared Shaw (UC Davis)