

ORGANIC CHEMISTRY 1 LECTURE GUIDE 2019

BY RHETT C. SMITH

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By Rhett C. Smith, Ph.D.

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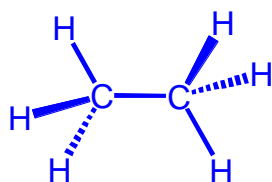
Organic Chemistry 1 Reactions and Practice Problems 2019

by Rhett C. Smith

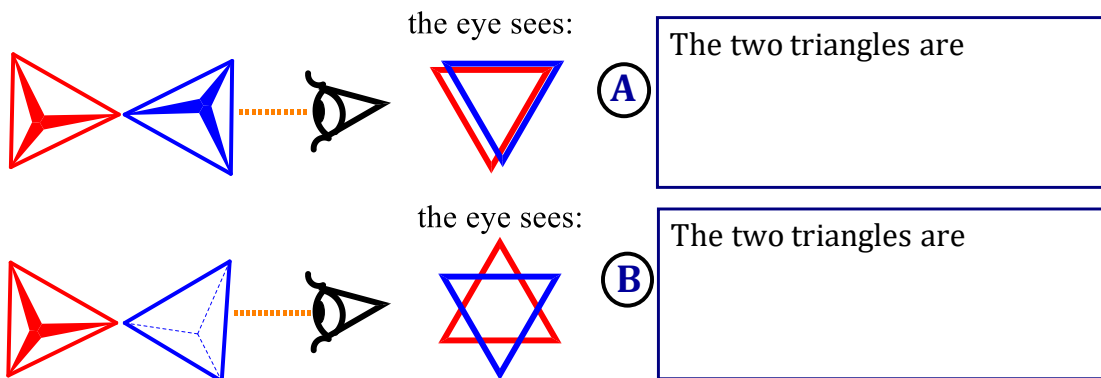
Organic Chemistry 1 Primer 2019,

by Rhett C. Smith, Andrew G. Tennyson, and Tania Houjeiry

Lecture Topic I.15: Isomerism and Conformational Analysis I
Rotating around a C-C Bond Leads to Different Conformations



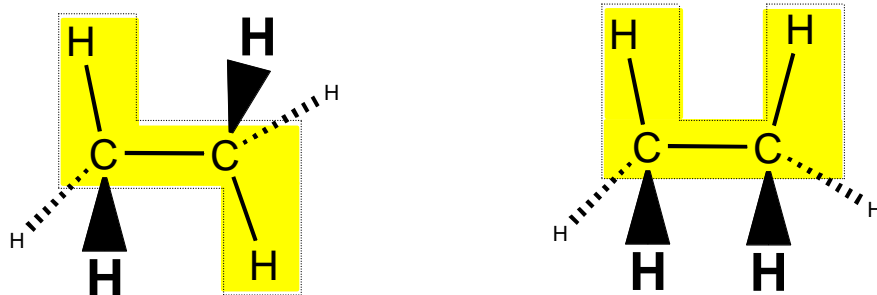
In ethane, two tetrahedral C are bonded to one another. We can think of this geometrically by joining two tetrahedra at a corner:



There are different **conformations** in which the two tetrahedra can be oriented with respect to one another, based on the relative rotation of the tetrahedral C atoms about the C-C bond.

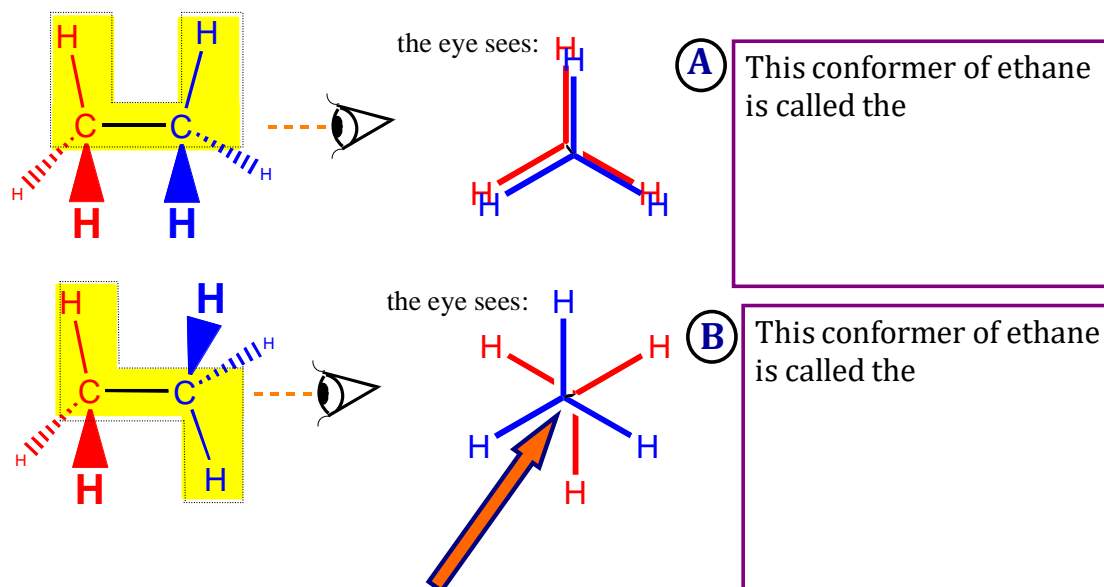
Notes

The use of wedges and hashed lines lets us represent the possible 3D shapes so we can visualize the possible **conformations**:



Notice in the left conformer the two H's coming out at us are far apart from one another, while in the right conformer they are right next to each other. These are two **conformational isomers** -

Notes



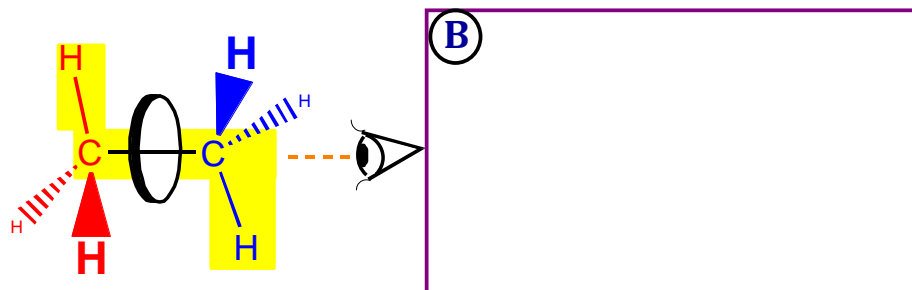
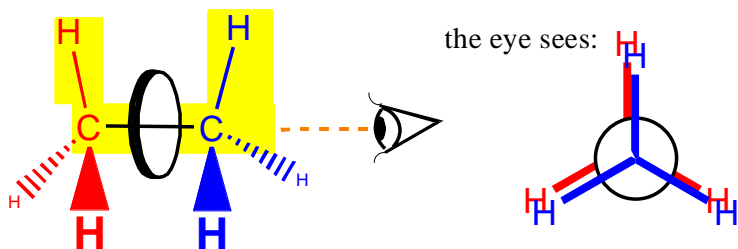
These representations emphasize the fact that we have two different conformers, but are a bit messy, especially at the middle, where all the bonds converge. For this reason, another way of representing this has been developed ...

Notes

Lecture Topic I.15: Isomerism and Conformational Analysis I
Newman Projections Conveniently Show Conformation

Put a disk in to block the view of the middle portion of the back, so that the middle is more tidy, and you get what are called

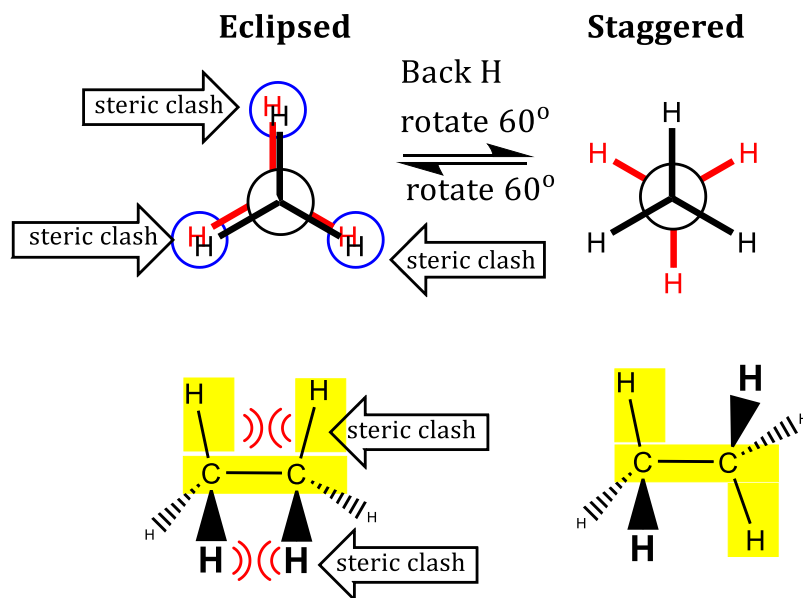
(A)



If you cut a little circle of paper, put in on your model kit ethane, and look from the end, you'll see exactly what the Newman Projection represents.

Notes

Lecture Topic I.15: Isomerism and Conformational Analysis I
Steric Repulsion Destabilizes Eclipsed Conformations

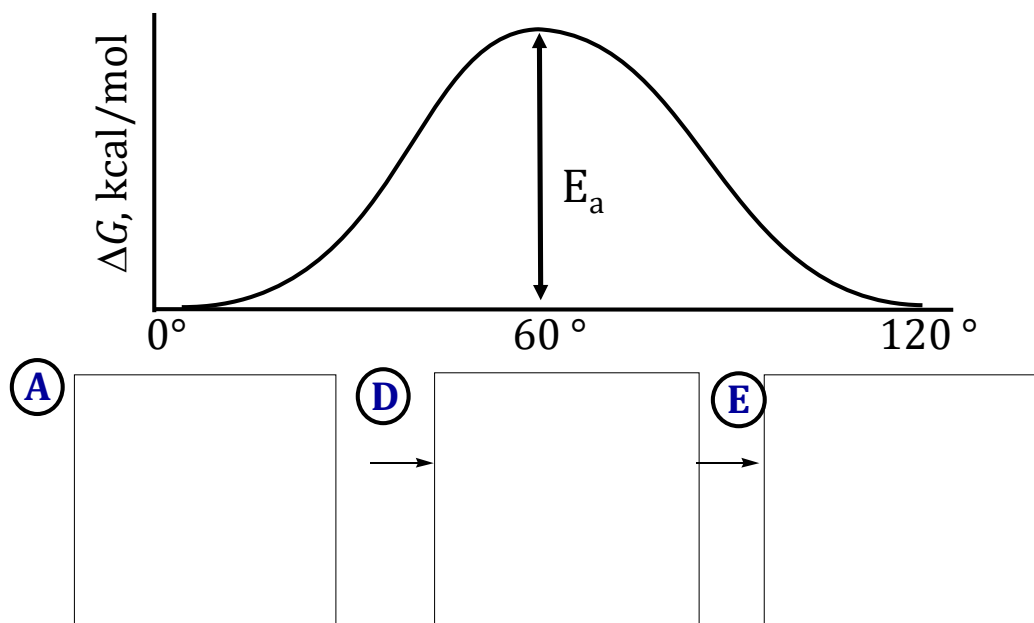


In the eclipsed conformation, H substituents are physically bumping into one another; such interactions are called **steric** interactions (steric interactions lead to different stereoisomers). In staggered, the H atoms are far apart. Because of sterics,

Notes

Lecture Topic I.15: Isomerism and Conformational Analysis I
Steric Repulsion Destabilizes Eclipsed Conformations

Steric clashes leads to an energy barrier (E_a) to rotation about the C-C bond. This energy barrier is called the **torsional strain** (resistance to twisting). Below is an energy profile showing how stability changes with bond rotation.

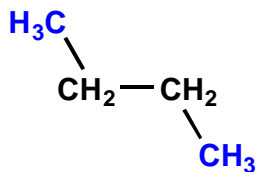


Notes

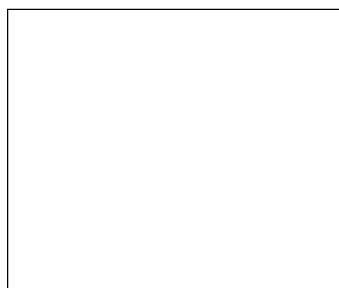
Lecture Topic I.15: Isomerism and Conformational Analysis I

Concepts to Analyze Ethane can be applied to other Molecules

Ethane is simple because we only have hydrogens on the C-C bond. Now we look at a more complicated example, butane.



Butane has both hydrogen and methyl groups attached to the C2-C3 bond. This leads to more possible stereoisomers than we saw with ethane ...



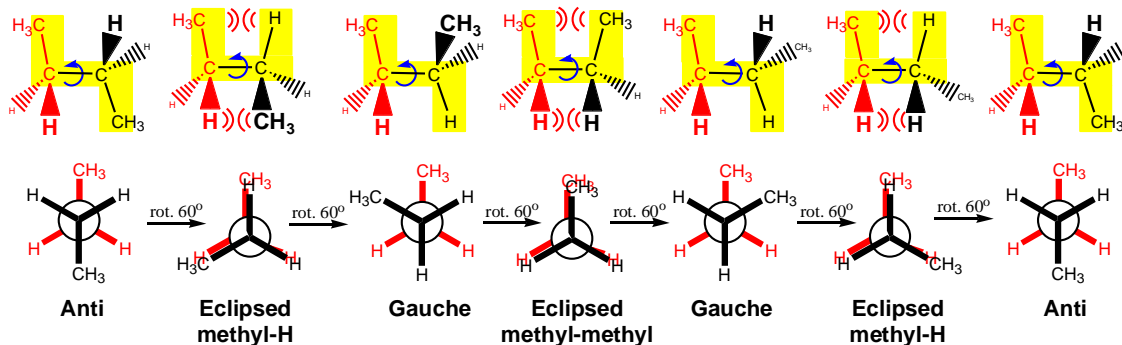
Ethane



Butane

Notes

Lecture Topic I.15: Isomerism and Conformational Analysis
 There are Four Staggered/Eclipsed Conformations of Butane



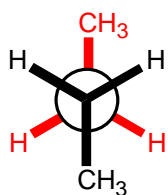
four distinct conformers:



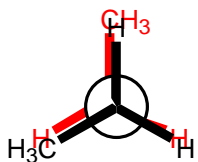
We can predict the relative stability of these conformations by evaluating the steric strain in each of them...

Notes

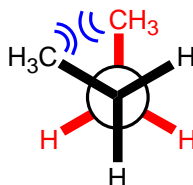
Lecture Topic I.15: Isomerism and Conformational Analysis I
Assessing Sterics Allows Prediction of Stability



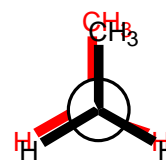
Anti



**Eclipsed
methyl-H**



Gauche



**Eclipsed
methyl-methyl**

Since methyl groups are larger than hydrogens,

A

In fact, two methyl groups have some steric repulsion even when they are still 60° apart from one another, a repulsion called a

B

Notes