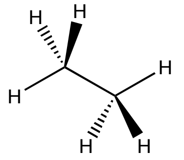
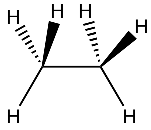
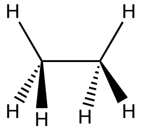
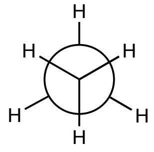
Structure, Conformations of Acyclic Alkanes (3.7)

A. "Conformations" = "Conformers" = "Rotamers" = different 3-D arrangements resulting from rotation around a single bond


Normal zig-zag

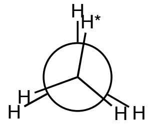


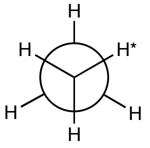

"sawhorse"

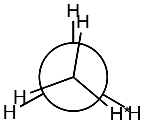

"Newman Projection"

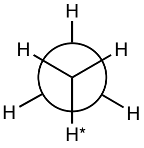
B. "Newman Projections": look straight down one C-C bond

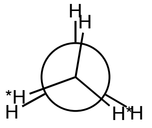
- If both bonded carbons are tetrahedral, there will be three bonds extending from the front carbon, and three more bonds extending from the back carbon
- Terms:
    - **Dihedral angle**: angle between a bond on the front atom relative to a bond on the back atom
    - **Eclipsed**: when bonds are aligned. 0º, 120º, 240º, 360º dihedral angles
    - **Staggered**: when bonds are as far apart as possible: 60º, 180º, 300º
    - **Skew**: anything else in between the eclipsed and staggered extremes

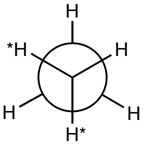

0º
eclipsed

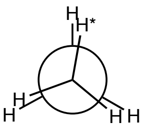

60º
staggered


120º
eclipsed


180º
staggered


240º
eclipsed


300º
staggered

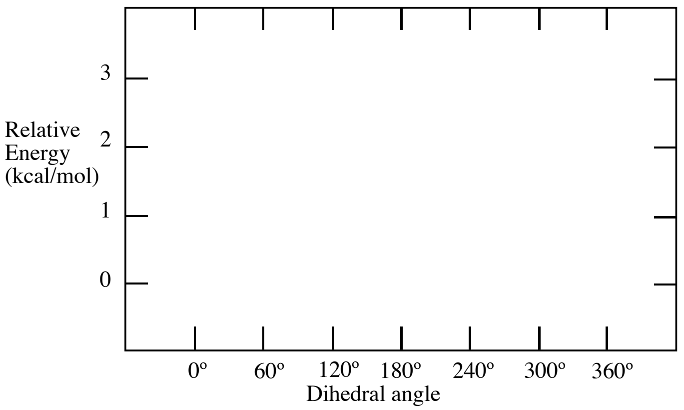

360º
eclipsed

Energy: **Staggered best, eclipsed worst**

- Why: Torsional strain. **Repulsion between bonding electron pairs** is reduced in the staggered conformation, and is worst in the eclipsed conformation.

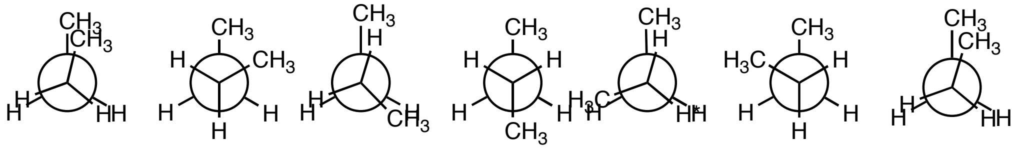
Rotation Barrier: energy gap between the best and worst conformation when you go through a full 360º rotation (as would take place in a full bond rotation)

- Draw in Entergy diagram:

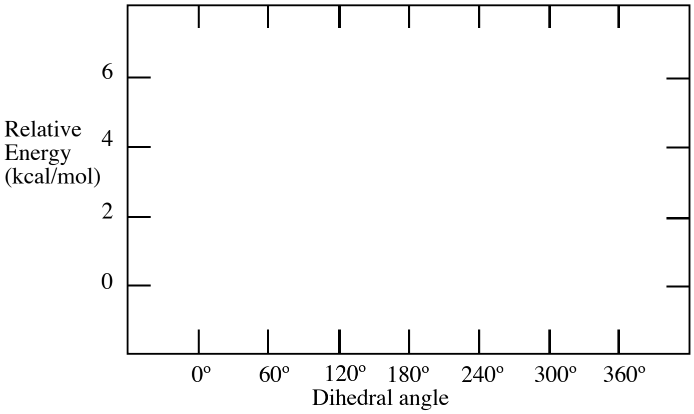


Conformations of Butane and Longer Alkanes (3.8)

CH_3CH_2-CH_2CH_3 is more complex. Focus down C2-C3 bond.



0° eclipsed	60° staggered	120° eclipsed	180° staggered	240° eclipsed	300° staggered	360° eclipsed
Totally Eclipsed	**Gauche**	**Eclipsed**	**Anti**	**Eclipsed**	**Gauche**	**Totally Eclipsed**
6.0	0.9	3.6	0	3.6	0.9	6.0



Questions

1. Draw the energy diagram

2. What would be the rotation barrier?

Strain Energy Factors:

1. **Torsional** strain (why all of the eclipsed type conformations are worse). Repulsion between bonded electrons
2. **Steric** strain: When atoms themselves get too close. Atom-atom repulsion.
3. **Angle** strain: When bond angles can't achieve ideal VSEPR angles. (No angle strain in ethane or butane)

Total Strain = Torsional strain (are any bonds eclipsed?)
+ Steric strain (are any atoms too close)
+ Angle strain (are any bond angles forced to be other than ideal?)

Questions

1. In general, why are staggered better than eclipsed?

2. Why is eclipsed better than totally eclipsed?

3. Why is anti better than gauche?

4. Why is gauche better than eclipsed?

5. Why is anti better than totally eclipsed?