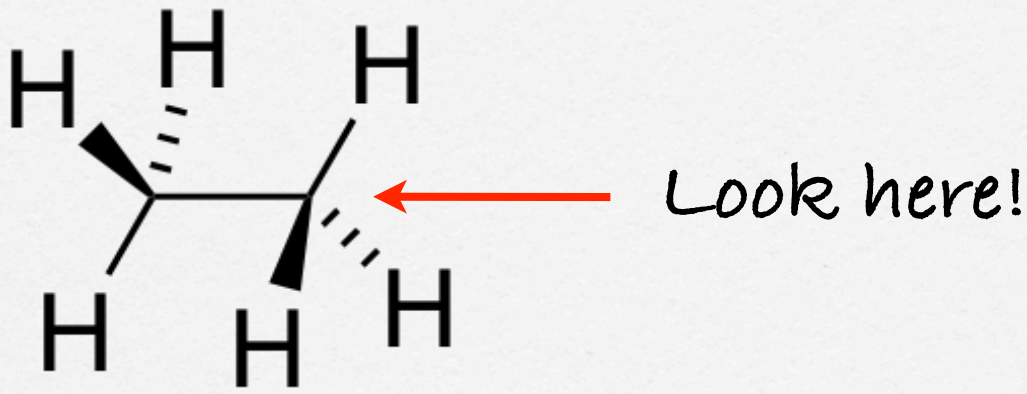
Acyclic Alkane Conformers

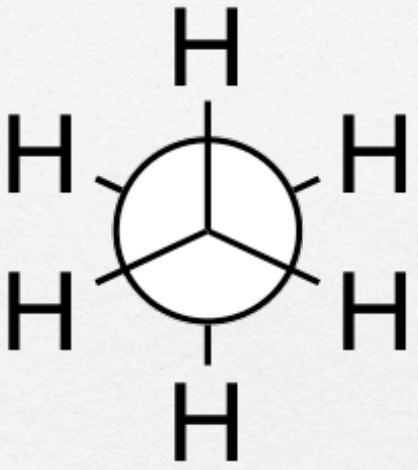
UCI Chem 51A
Dr. Link

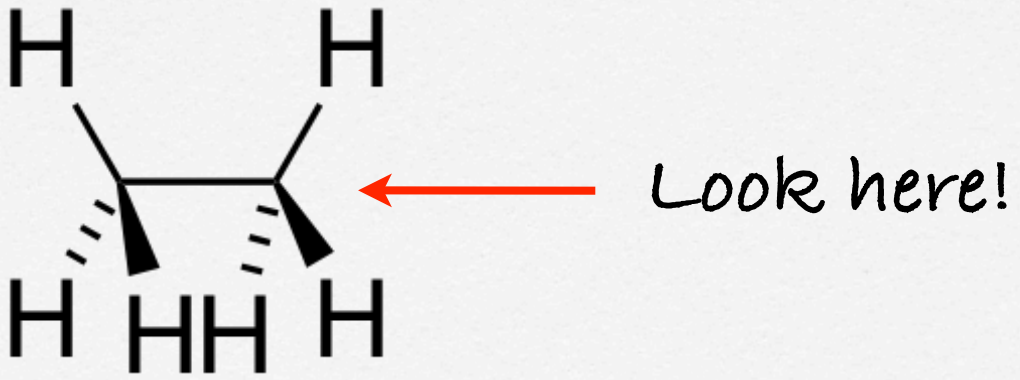
Goals

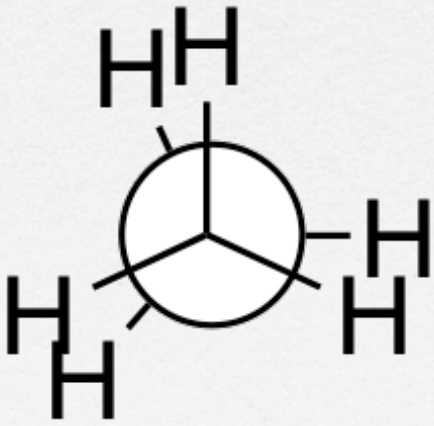
- After this lesson you should be able to
  - Identify the types of strain present in different conformers of an acyclic molecule
  - Estimate the quantity of strain present in a particular conformer
  - Qualitatively compare the relative energies of different conformers
  - Draw Newman projections for acyclic molecules

Ethane 3D

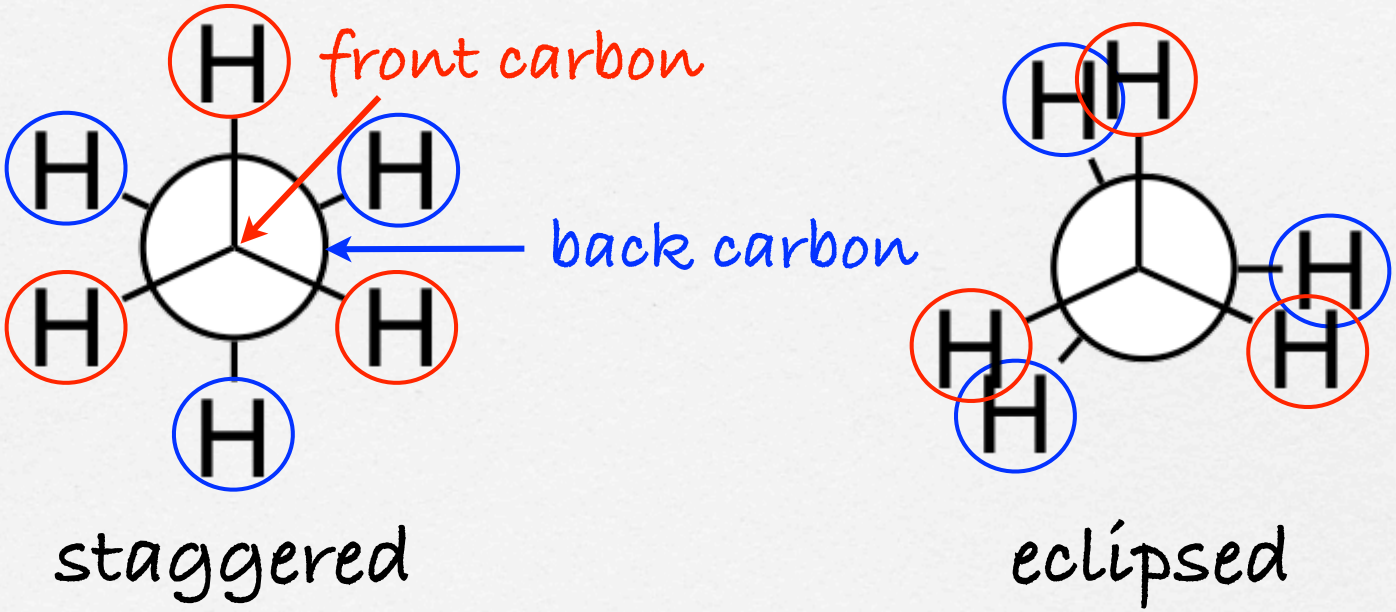








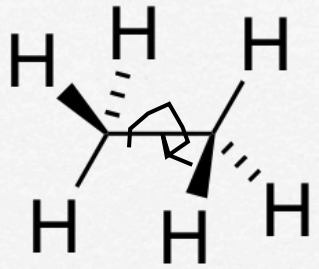
Newman Projections



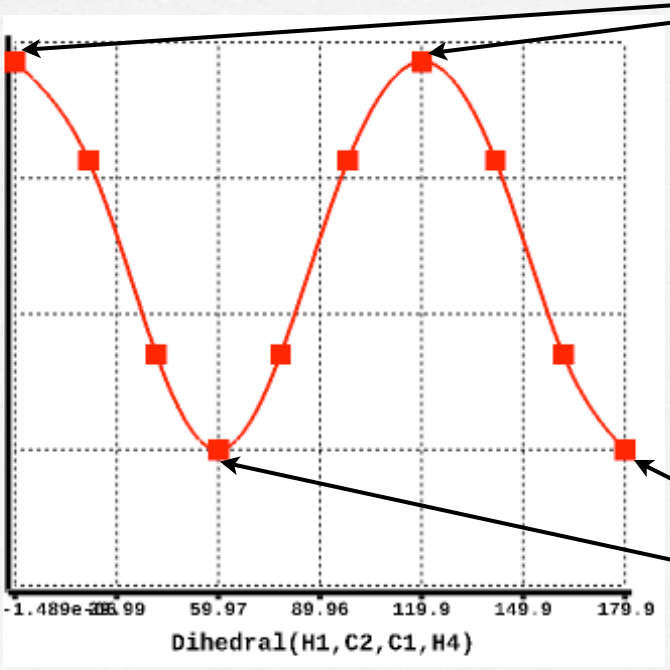
How to Draw A Newman Projection

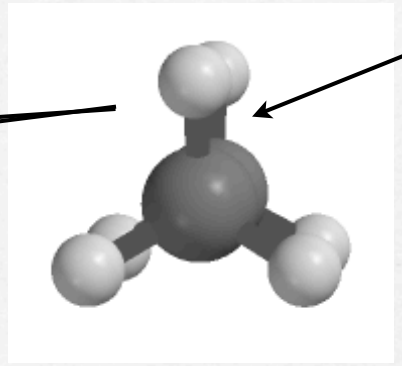
- 1. Choose a bond to look down
- 2. Identify front and back atoms
  - Front = dot
  - Back = circle
- 3. Draw in bonds as shown (Bonds to front atom should cross over circle of back atom.)
- 4. Add atoms to bonds
- **Use models to start! Draw EXACTLY what you see!

Back to Ethane

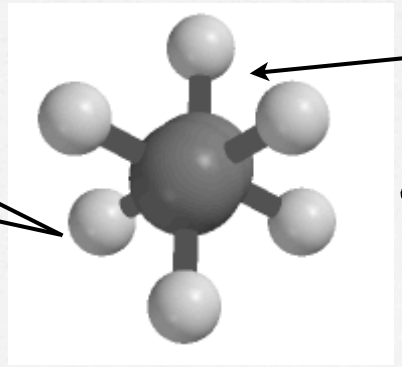


- Rotation around bonds!





dihedral angle 0°, 120°, etc.

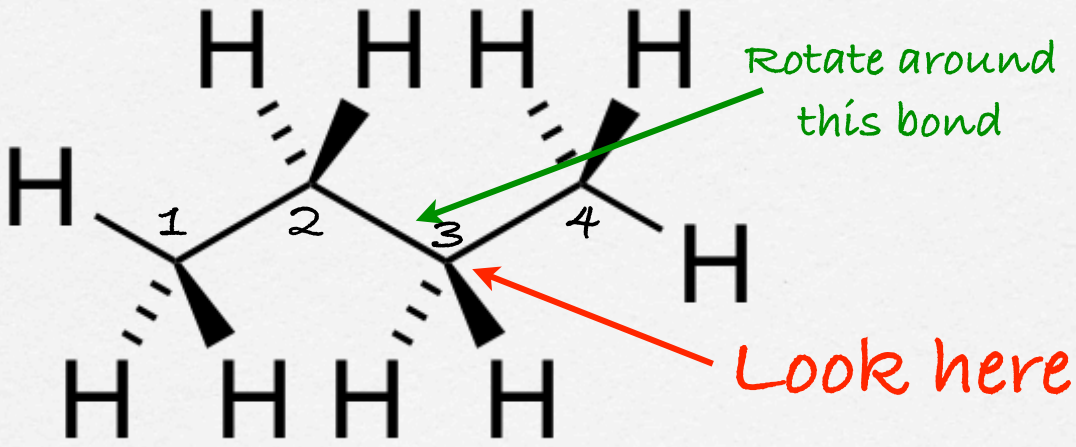


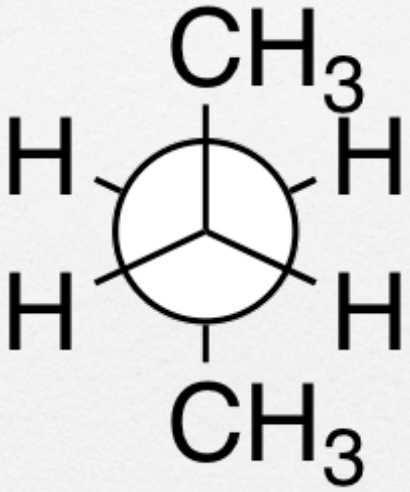
dihedral angle 60°, 180°, etc.

Types of Strain

- angle strain: increase in energy when angles deviate from optimum angle
- torsional strain: increase in energy caused by eclipsing interactions
- (one more soon!)

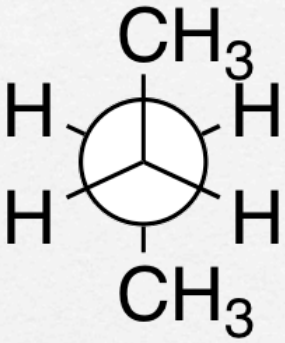
Butane 3D





What other conformers can we draw?

Back to Newman Projections



staggered
anti

rotate
60°

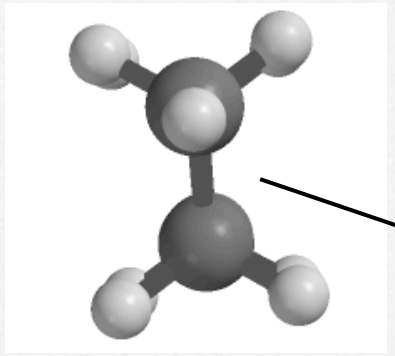
rotate
60°

rotate
60°

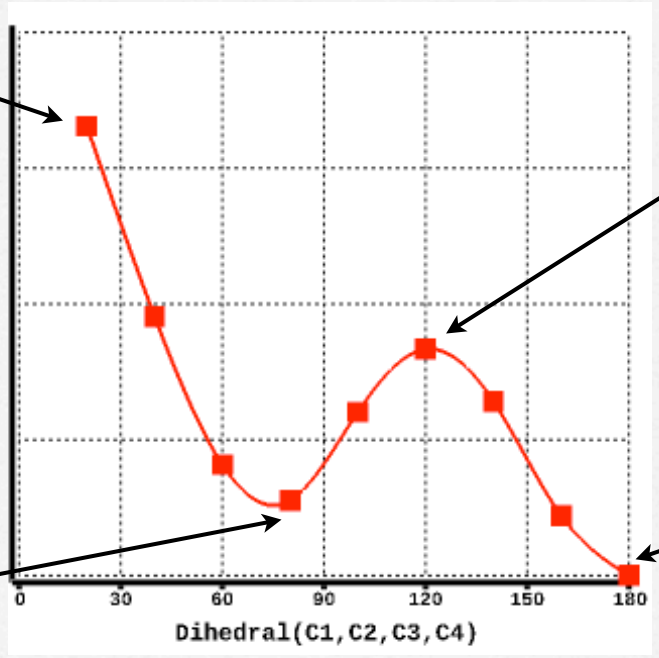
rotate
60°

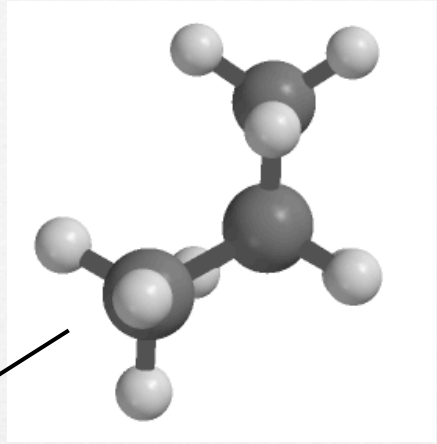
and
so on...

Energy Profile

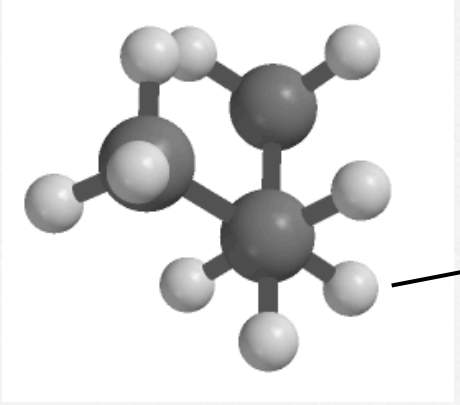


CH_3-CH_3
eclipsed

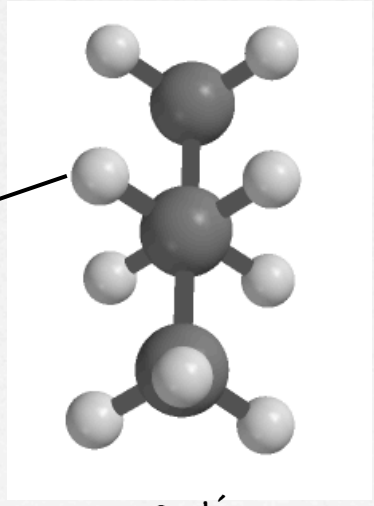




CH_3-H
eclipsed



gauche



anti

Energy Costs

Eclipsing

Interaction	Energy Cost
Eclipsing H-H	
Eclipsing CH_3-H	
Eclipsing CH_3-CH_3	

Gauche

Interaction	Energy Cost
Gauche H-H	0 kcal/mol
Gauche CH_3-H	0 kcal/mol
Gauche CH_3-CH_3	

- When comparing conformers, look for the differences in interactions rather than all interactions!

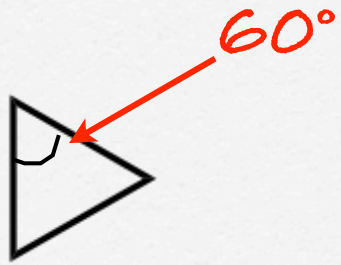
*relative energies. Gauche H-H set as zero

Types of Strain

- angle strain: increase in energy when angles deviate from optimum angle
- torsional strain: increase in energy caused by eclipsing interactions
- steric strain: increase in energy caused when atoms are brought too close to each other

Strain Visuals

Angle Strain

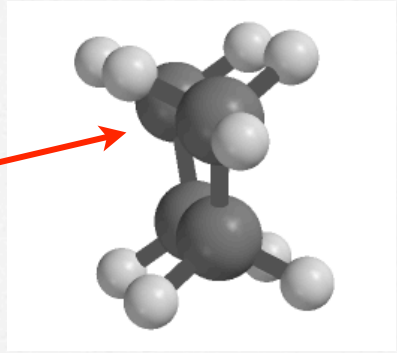


60°<109.5°

Costs energy!

Torsional Strain

eclipsing interaction



e^- densities line up, repel

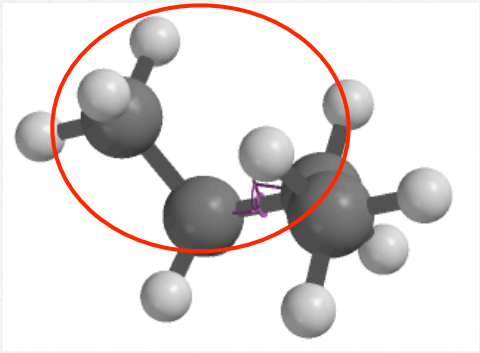
Costs energy!

Strain Visuals: Steric Strain

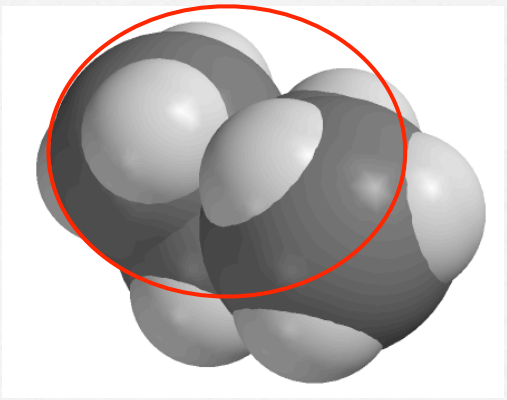
Steric Strain

hydrogens on CH_3's trying to occupy same space

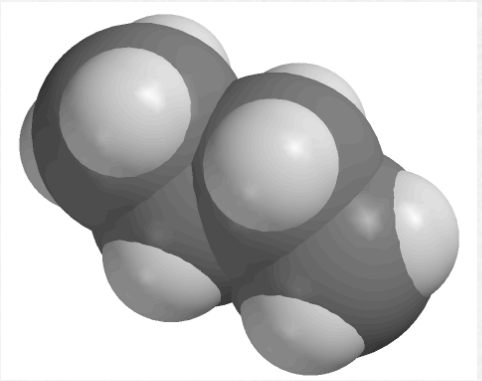
CH_3's pointing away from each other



gauche conformer



gauche conformer



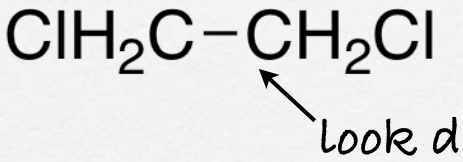
anti conformer

So What Does Butane REALLY Look Like?

- Anti?
- Gauche?
- Eclipsed?
- ALL OF THE ABOVE! Bonds rotate!
  - At 20 °C, ~70% anti, ~30% gauche, <1% eclipsed (total)
- Physical properties observed are a combination of the properties of different conformers.

Conformer Practice

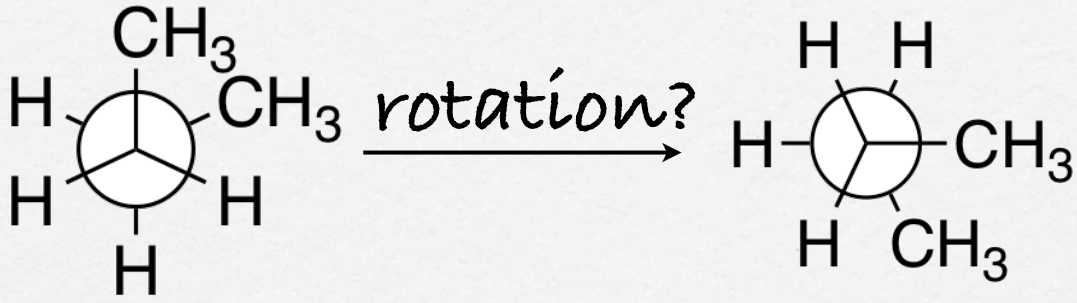
- What would be the highest and lowest energy conformers for 1,2-dichloroethane?

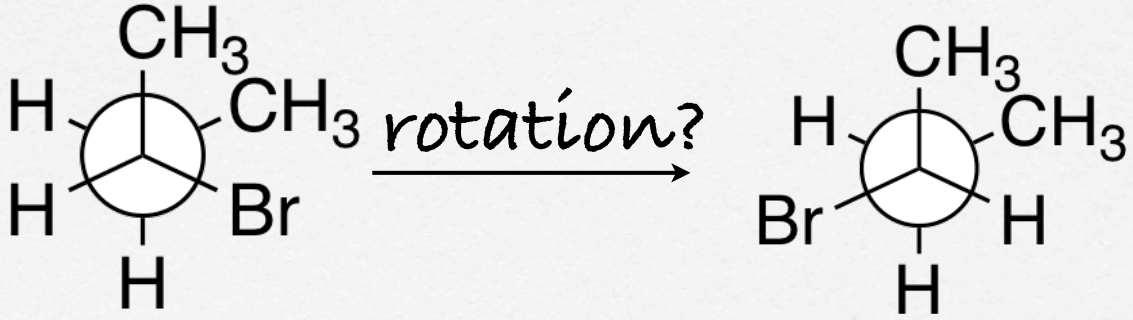


look down C-C bond

*No wedges or dashes drawn, so choose for yourself.

Common Newman Projection Mistakes





Wrapping Up

- Practice converting between skeletal structures and Newman projections
- Practice rotating in Newman projections
- Practice ranking conformers of a molecule by relative energies
- Practice recognizing types of strain present in each conformer