

Team Poster Activity: To Rotate or Not to Rotate

Always often means 'most of the time' and

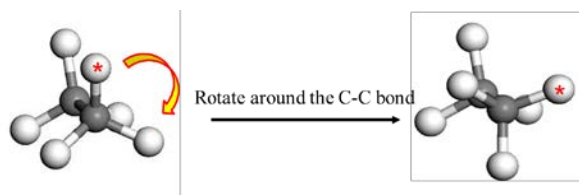
Never often means 'not usually'

Although the connectivity of atoms in a molecule is relatively fixed by the strength of bonds, molecules are, nevertheless, in dynamic motion. The atoms vibrate as bonds lengthen and shorten and as bond angles change around their average values (*i.e.* the average bond lengths and angles). The atoms at one end of a bond may also rotate with respect to atoms at the other end. The extent of motion often depends on the temperature with higher temperatures leading to greater motion.

In class we spoke of "rotation around a single bond" as if it always occurred, and "no rotation around a double bond" as if it never occurred. In this activity you will ask, "Are there molecular situations where the 'always' and 'never' do not hold?" To explore this question, your team will make a poster that addresses, *in your own (team's) words*, each of the questions below. Before meeting with your team to create your poster: **Go over each of the following questions that are based on observations you make using the following interactive molecular viewer links: [Q1-Q2, Q3 (a,b,c), Q4 (a,b,c,d)].** Bring your observations and conclusions to your team's poster session!!

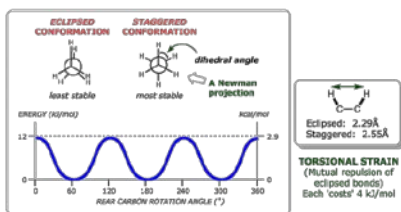
In this activity, you will apply your knowledge of hybridization to explore novel phenomena and attain a deeper understanding of bonding in polyatomic molecules.

Q1: What hybrid orbitals form the C—C bond in the molecule, ethane (CH_3CH_3) and why are the two CH_3 groups 'free' to rotate around the C—C bond?

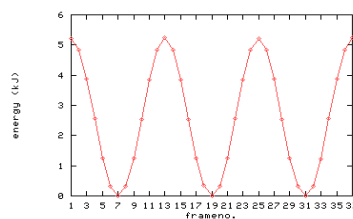


Q2: As the CH_3 groups rotate are they really 'free'?; do all positions of the CH_3 groups have the same energy?; why or why not?

In each of the demonstrations (I. and II.) there is a diagram with hills and valleys:



(from URL I)



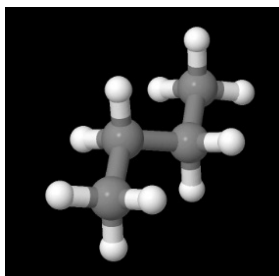
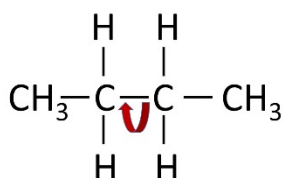
(from URL II requires JAVA)

The energy of the ethane molecule is plotted on the y-coordinate, but

- What is being plotted on the horizontal axis?
- What molecular geometry (conformation) of ethane corresponds to the 'top of the hill'? and
- What conformation corresponds with the 'bottom of the valley'?

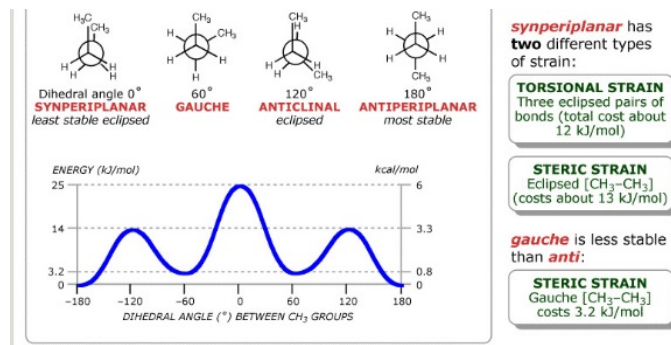
Q3: What are conditions where the two ends of a molecule might NOT be able to freely rotate around a single C—C bond?

- Are there physical conditions where the ethane molecule might be 'trapped' in the geometry that corresponds to geometries near the bottom of the valley?
- Are there structures where rotation around the single bond may be more hindered than that in ethane? Consider rotation around the central bond in butane in your answer:

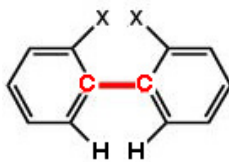


grey spheres – C
white spheres – H

The 'hill and valley' diagram for rotation around this bond is:



- Why do the "hills" for rotation around the central C—C bond in butane (CH₃CH₂CH₂CH₃) have differing heights?
 - Notice for the rotation in butane, the 'top of the high hill' is 25 kJ/mol, while for ethane it is only 12 kJ/mole. Explain the reason for this difference.
- c. The molecule below is called a substituted "diphenyl". Various atoms can be substituted at the positions marked X.



- What hybrid orbitals interact to form the central C—C bond?
- What would be a characteristic of an atom at position X that would hinder free rotation around the C—C 'single' bond and favor non-planar conformations?
- Would a diphenyl with X = H or X = Cl be less likely to 'freely rotate'?
- BRAINIAC QUESTION: *The fact that each of the C's participating in the bond also has unhybridized $2p\pi$ orbitals actually makes the situation 'more interesting'. Can you suggest how the presence of these unhybridized $2p\pi$ orbitals would 'favor' a planar conformation?*

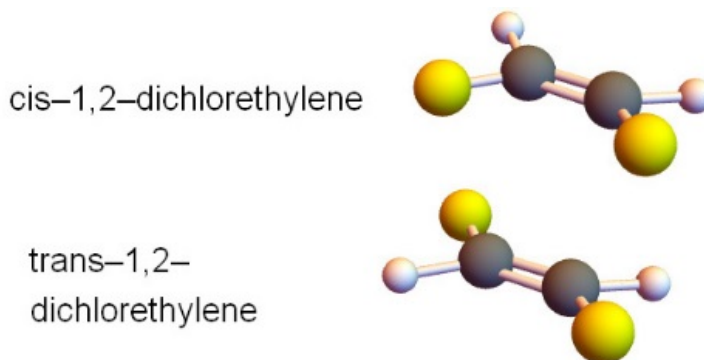
Q4

a. Why in the molecule ethene (ethylene) CH_2CH_2 are the two CH_2 groups 'not free' to rotate around the C=C bond in the ground electronic state?

- Draw the energy level diagram for the four MOs involved in the C=C double bond and indicate their occupancy in the ground electronic state of ethylene.
- Rotation around the C=C would require the 'breaking' of which of the two occupied orbitals? *i.e.* which of the two types of bonds constituting the double bond needs to be broken before rotation?

b. How might one initiate a cis- to trans- rotation around the C=C double bond?

- What excited state electronic configuration would weaken the double bond (give 'no bonding')?
- How might a molecule like ethylene achieve this excited state?



[see it happen !!](#)