

Hybridization Theory: Understanding Molecular Geometry

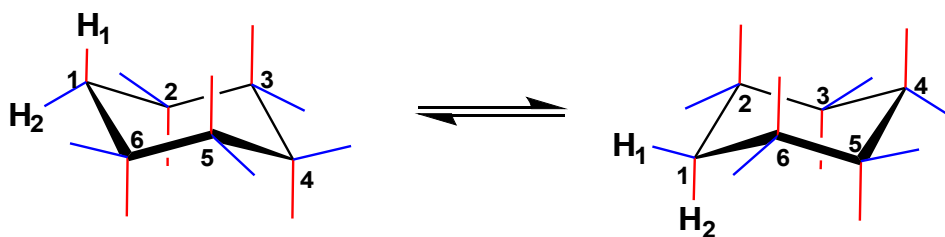
Key Terms:

abbreviated electron configuration – combines the inert, noble core electrons (abbreviated via a noble element) with the outermost or valence electrons allowing the student to quickly ascertain the number of valence electrons.

atomic orbitals - three-dimensional shapes where you are most likely to find an electron 90% of the time.

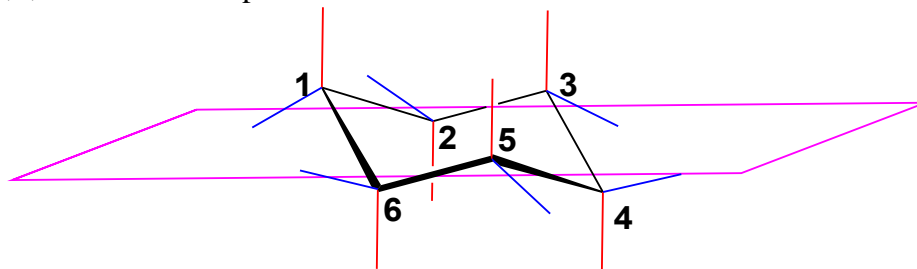
axial/equatorial position(s) – When a cyclohexane ring is in the most stable conformation, a chair, six of the twelve hydrogens are oriented around the perimeter of the ring much like the equator around earth. These hydrogens are called equatorial hydrogens and are colored in blue. The other six hydrogens are parallel and are oriented straight up and down, called axial hydrogens. The axial hydrogens are shown in red and are much like the axis that goes through planet earth. It is worth mentioning that as the cyclohexane ring converts between both chair conformations, called ring-flipping or chair conversion, that the equatorial hydrogen becomes axial and the axial hydrogen becomes equatorial.

Chair Conformations



Cahn-Ingold Prelog sequence rules – a set of rules which allow one to deduce groups of priority on double bonds or stereocenters, which is usually deduced via differences of molecular weights.

chair conformation - the most stable conformation for a six-member (cyclohexane) ring. Because all six carbons are sp^3 hybridized the ring can't be in a planar arrangement (shown in purple) due to the ideal bond angle of 109.5° ; thus, the ring is puckered as shown and is called a chair conformation. Note that carbon-1,3,5 are above the plane and carbon-2,4,6 are below the plane.



cis and trans isomer - when we draw an imaginary line along the axis of the double bond and then compare groups on each carbon using the Cahn-Ingold Prelog sequence rules, we can determine if the groups of priority are on the same side, called the *cis* isomer, often abbreviated Z. Alternatively, the groups of priority can be on opposite sides of the imaginary line called the *trans* isomer, often abbreviated E.

conformation – due to rotation(s) about sigma bonds atoms can be oriented in space in an infinite way; however, the lowest energy arrangements are preferred. When the atoms are in a particular arrangement in space at some time, t , we call this a conformation.

covalent bond – when two atoms share a pair of electrons in an attempt to gain stability. The difference of electronegativity values between these two atoms should not exceed 2.1 or a transfer of electron(s) will occur leading to an ionic bond.

degenerate-energy – same as stating, “equal in energy.”

dihedral angle – angle created between two groups that are attached to adjacent atoms.

eclipsed conformation – when groups on two adjacent sp^3 hybridized carbon atoms overlap when viewed down the sigma bond; i.e., a Newman projection (usually the highest energy conformation).

electron configuration – indicates where all the electrons are located for an atom; the principle quantum number, the orbital, and how many electrons are in each orbital via superscripts.

equatorial position(s) – see axial position(s).

full valency - a term often employed when an atom has gained electrons to become isoelectronic with a noble element; usually adhering to the octet or duet rule.

geometric isomers - have the same gross connectivity but differ only how the groups are oriented in space due to hindered rotation about the doubly-bonded carbons. In addition, geometric isomers also have different chemical and physical properties.

hybrid orbitals - a mixture of two or more different shape atomic orbitals.

inert – unreactive, not involved in bond making or breaking.

Newman projection - when the molecules are viewed down the C-C sigma bond.

noble core electrons – a set of electrons that are isoelectronic with a noble element. Because these inner-core electrons are not involved in bond making or breaking they are normally abbreviated as a noble element (in brackets) for convenience.

pi (π) bond – overlap of adjacent, parallel p orbitals above and below a plane.

sigma (σ) bond - electron density is symmetrically located about an imaginary line that runs between the two adjacent nuclei

staggered conformation - when groups on two adjacent sp^3 hybridized carbon atoms do not overlap when viewed down the sigma bond; i.e., a Newman projection (usually the lowest energy conformation).

steric factor – a spacial, physical impedance.

structural isomers – arise when two structures share the same molecular formula but different gross connectivity. In addition, structural isomers have different chemical and physical properties.

tetravalent carbon – carbon that has the ability to form four sigma bonds.

torsional strain – electrons that are found in adjacent bonds cause an electrostatic repulsion, which is a destabilizing effect.

valence electrons – the outermost electrons involved in bond making and bond breaking.

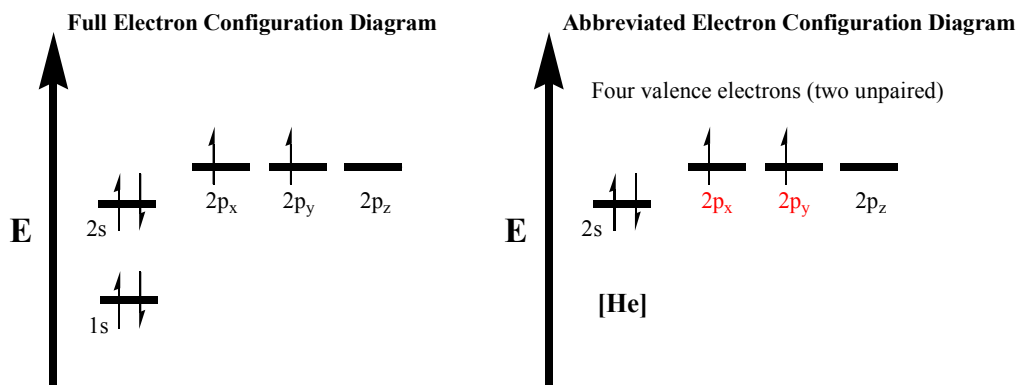
VSEPR - valence shell electron pair repulsion theory, allows the chemist to make predictions regarding deviations from ideal bond angles.

Chapter One Questions:

- 1) What are some of the advantages for the chemistry student who understands hybridization theory?
- 2) Examining the abbreviated electron configuration for an atom allows the chemist to quickly determine the number of valence electrons. How many valence electrons does carbon have?
- 3) How many unpaired electrons does an atom of carbon have in its ground state?
- 4) How many bonds will carbon form to attain full valency?
- 5) Which electrons are responsible for bond making and bond breaking?
- 6) Write the full electron configuration for a neutral atom of carbon.
- 7) Draw the relative energy electron configuration diagram for a neutral atom of carbon.
- 8) What does each half arrow represent in the relative energy electron configuration diagram?
- 9) Why are two-dimensional Lewis diagrams important?
- 10) What are the possible hybridizations for an atom of carbon?

Chapter One Answers:

- 1) The chemistry student who has the ability to visualize molecules in three-dimensions is rewarded with a better understanding of chemical properties, physical properties, and most importantly, the ability to predict chemical reactivity.
- 2) The abbreviated electron configuration quickly allows one to ascertain that there are four valence electrons for carbon.
- 3) There are two unpaired valence electrons for carbon, one in the $2p_x$ and one in the $2p_y$ orbital.
- 4) Carbon forms a total of four covalent bonds to attain full valency.
- 5) The valence, or outermost, electrons are responsible for bond making or bond breaking.
- 6) A carbon atom has six electrons in the following configuration, $1s^2 2s^2 2p^2$.
- 7) The relative energy electron configuration diagram for a neutral atom of carbon:



- 8) Each arrow in relative energy electron configuration diagram represents one of the individual electrons of carbon.

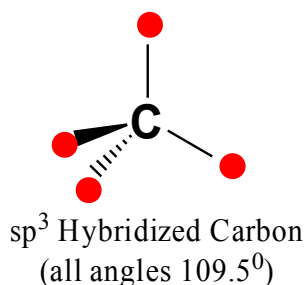
- 9) A two-dimensional Lewis structure of a molecule affords much information to the scientist; for example, gross connectivity of atoms within the molecular formula. After all, different structural and geometric isomers can be imagined from relatively simple molecular formulas.
- 10) The possible hybrid combinations for a carbon atom are sp^3 , sp^2 , and sp .

Chapter Two Questions:

- 1) What are the shapes of the 2s and 2p atomic orbitals?
- 2) What is the simplest way to explain the atomic orbitals?
- 3) Please describe the shape of the sp^3 hybridized orbital.
- 4) Please draw the sp^3 hybridized building block for an atom of carbon.
- 5) What are the angles of a sp^3 hybridized carbon atom?
- 6) Draw methane, CH_4 , in three-dimensions indicating bond angles.
- 7) Compare the bond angles within the two-dimensional Lewis structure for ethane with the bond angles within three-dimensional structure for ethane employing the concepts of hybridization theory.
- 8) What type of bond allows for free rotation between adjacent carbons?
- 9) Draw in three-dimensions the staggered and eclipsed conformations of ethane indicating which is higher and lower in energy.
- 10) Draw the Newman projections for the staggered and eclipsed conformations of ethane.

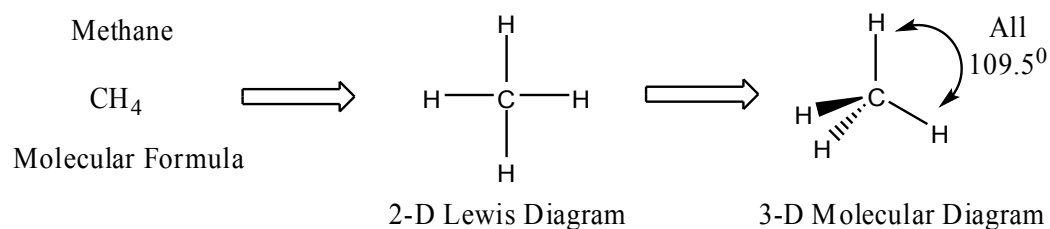
Chapter Two Answers:

- 1) The 2s atomic orbital is a sphere and the three 2p atomic orbitals are shaped like dumb-bells oriented along the three axes; $2p_x$, $2p_y$, and $2p_z$.
- 2) Think of the atomic orbitals as three-dimensional shapes where you are most likely to find an electron 90% of the time.
- 3) The shape of the sp^3 hybrid orbital is best characterized as one part s and three parts p.
- 4)



- 5) The four new hybrid orbitals attempt to get as far apart from each other as possible to minimize electron repulsions. Thus, they are oriented toward the corners of a tetrahedron with all angles at 109.5° .

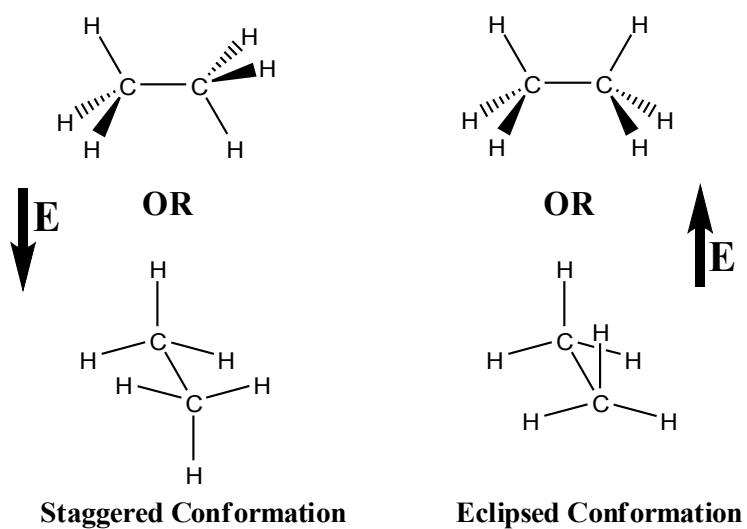
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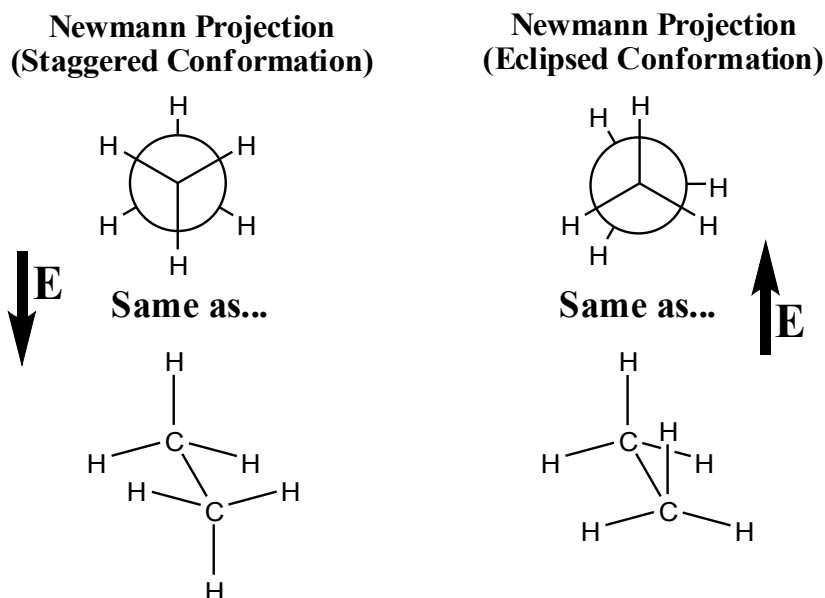
7) The two-dimensional Lewis diagram for ethane implies that all the bond angles are 90° . However, employing the basic principles of hybridization theory, we see that the bond angles are all nearly 109.5° .

8) Free rotation may occur about the C-C single bond, which is called the sigma bond.

9)



10)

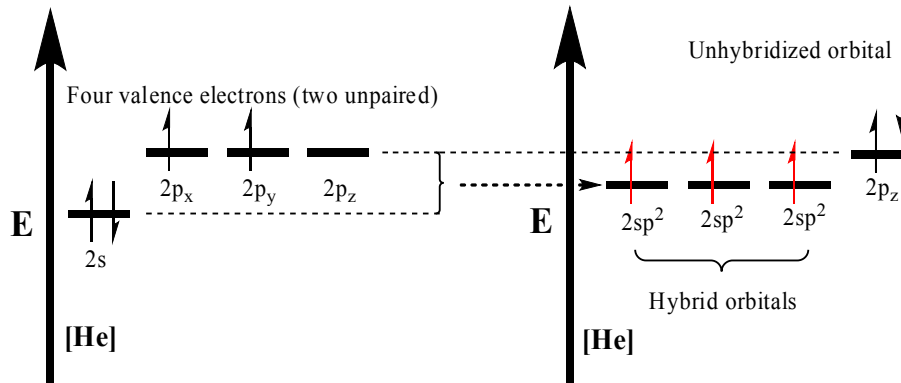
**Chapter Three Questions:**

- 1) Please describe where the valence electrons are located in an sp^2 hybridized carbon.
- 2) Please draw the abbreviated relative energy electron configuration diagrams for carbon and the sp^2 hybridized carbon.
- 3) Please describe the shape of the sp^2 hybridized orbital.
- 4) Please draw the sp^2 hybridized building block for an atom of carbon.
- 5) What are the angles of a sp^2 hybridized carbon atom?
- 6) Draw ethylene, C_2H_4 , in three-dimensions.
- 7) Please describe the difference between the *cis* and *trans* geometric isomer.
- 8) Please describe why most isomers are isolable at room temperature.

Chapter Three Answers:

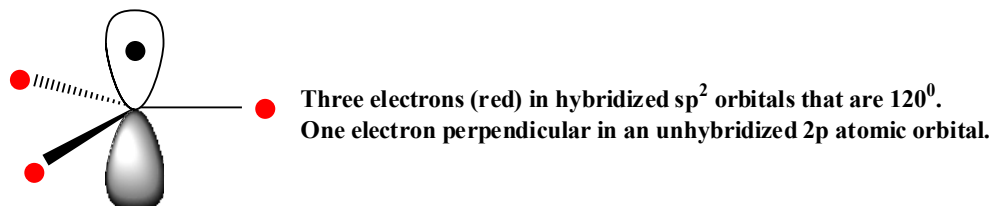
- 1) The sp^2 hybridized carbon possesses three electrons in hybrid orbitals and one electron in an unhybridized $2p$ orbital.

2)



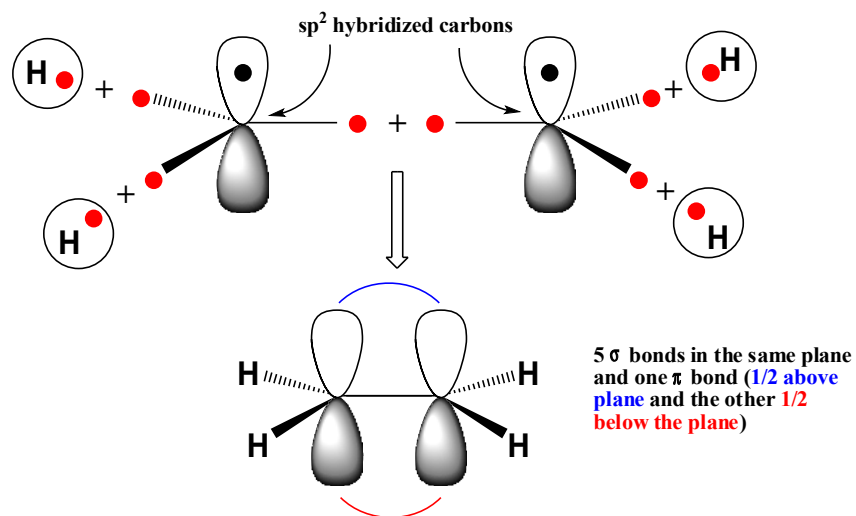
3) The shape of the sp^2 hybrid orbital is best characterized as one part s and two parts p.

4)



5) The three new hybrid orbitals attempt to get as far apart from each other as possible to minimize electron repulsions. Thus, the bond angles are 120° .

6)



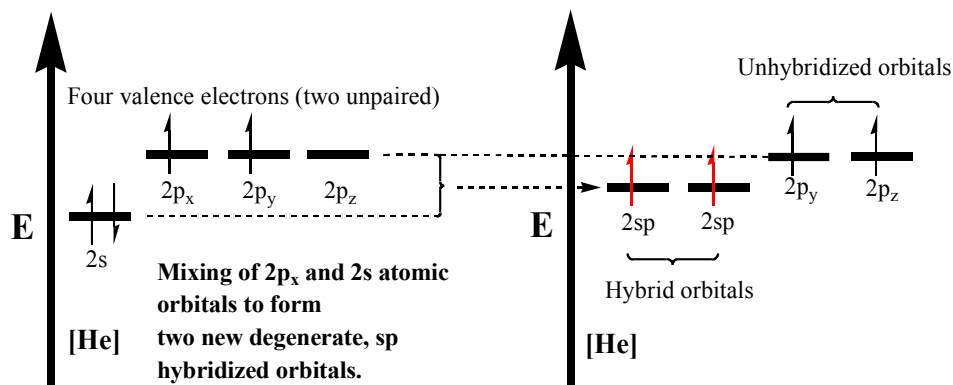
- 7) If the groups of priority are on the same side, called the *cis* isomer, often abbreviated Z. Alternatively, the groups of priority can be on opposite sides of the imaginary line called the *trans* isomer, often abbreviated E.
- 8) For interconversion of the isomers to occur we need to have free rotation about the C=C double bond. If this were to happen it would mean that the pi bond would have to break, which requires approximately 70 kcal/mol. This will cause each carbon to lose full valency due to the 2p orbitals no longer overlapping, which will make the alkene unstable or higher in relative energy. Thus, at room temperature geometric isomers are isolable.

Chapter Four Questions:

- 1) Please describe where the valence electrons are located in a sp hybridized carbon.
- 2) Please draw the abbreviated relative energy electron configuration diagrams for carbon and the sp hybridized carbon.
- 3) Please describe the shape of the sp hybridized orbital.
- 4) Please draw the sp hybridized building block for an atom of carbon.
- 5) What are the angles of a sp hybridized carbon atom?
- 6) Draw acetylene, C₂H₂, in three-dimensions.
- 7) How many sigma bonds can a sp hybridized carbon form?
- 8) How many pi bonds can a sp hybridized carbon form?

Chapter Four Answers:

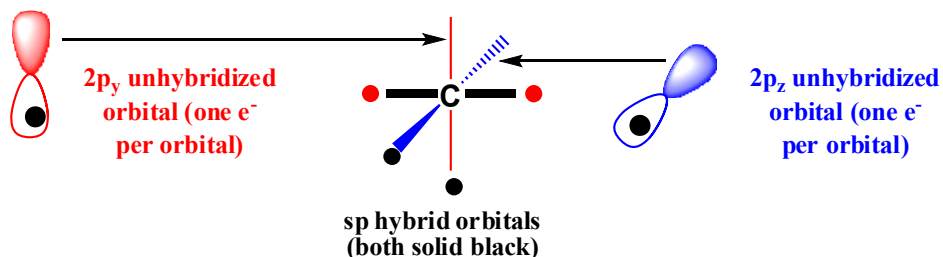
- 1) The sp hybridized carbon possesses two electrons in hybrid orbitals and two electrons in unhybridized 2p orbitals.
- 2)



- 3) The shape of the new sp hybrid orbital is best characterized as one part s and one part p.

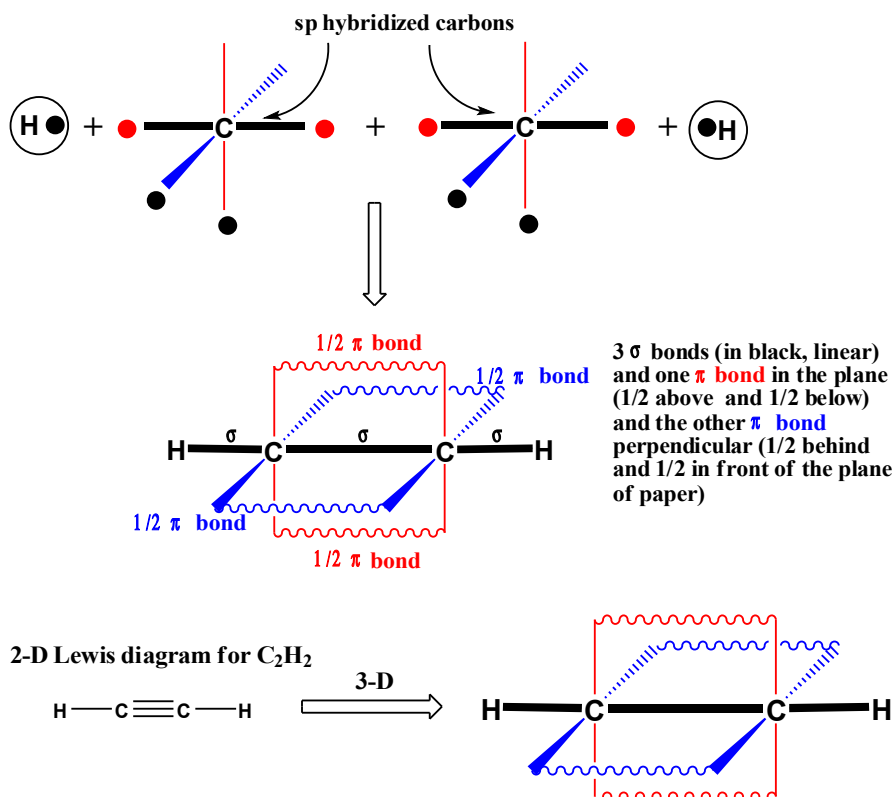
4)

Two electrons (red) in hybridized sp orbitals that are 180° .
 Two electrons perpendicular in unhybridized $2p$ atomic orbitals.



5) The two new hybrid orbitals attempt to get as far apart from each other as possible to minimize electron repulsions. Thus, the bond angles are 180° .

6)



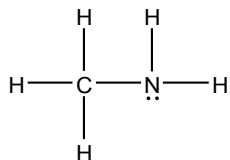
7) A sp hybridized carbon can form two sigma bonds, which will be 180° apart.

8) A sp hybridized carbon can form two pi bonds.

Chapter Five Questions:

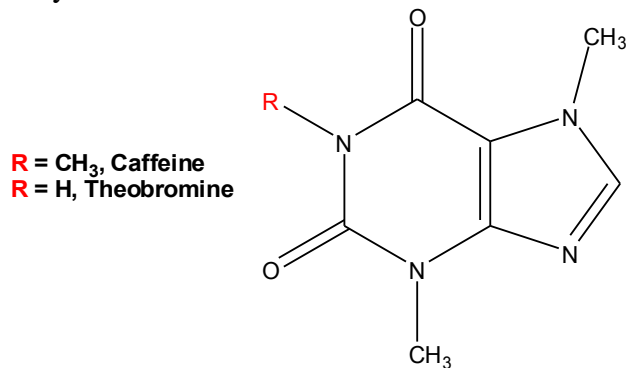
1) Please draw a sp^3 , sp^2 , and a sp hybridized carbon atom.

- 2) Please indicate the hybridization of each central atom in the following structure:

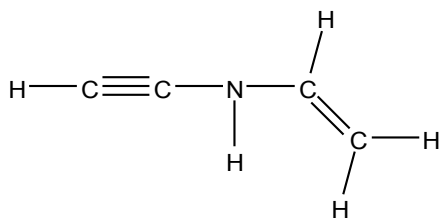


Methylamine

- 3) Please draw the structure in problem #2 in three-dimensions.
 4) Please indicate the hybridization of each central atom in the following structure:



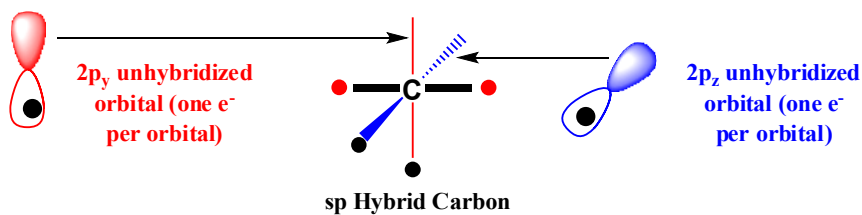
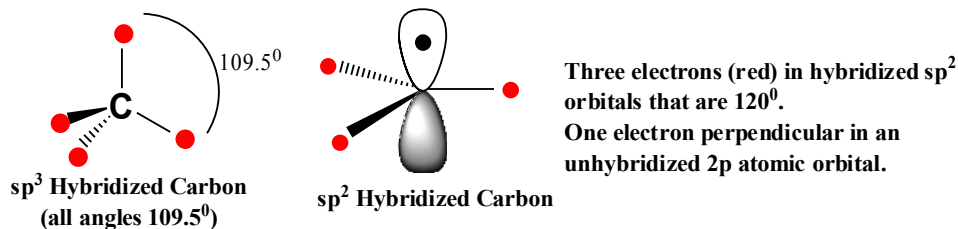
- 5) Please indicate the hybridization of each central atom in the following structure:



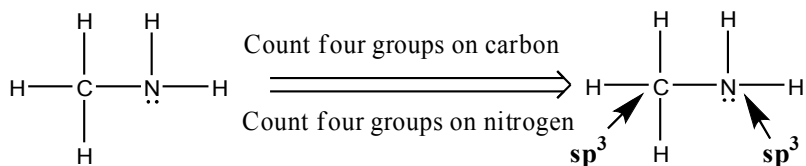
- 6) Please draw OF₂ in three-dimensions and indicate any deviations from ideal bond angles.

Chapter Five Answers:

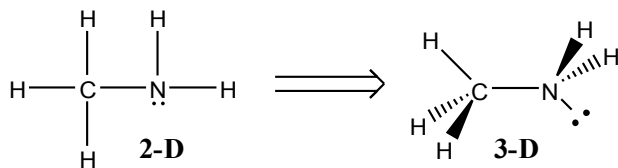
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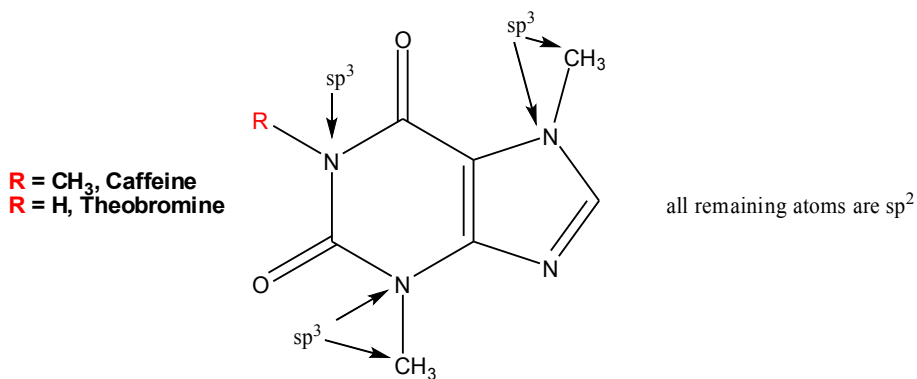
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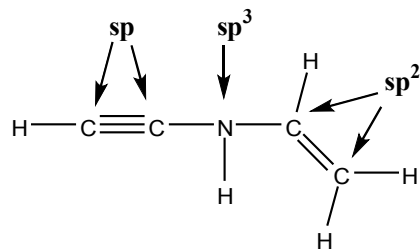
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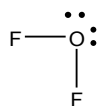
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5)



6)

 OF_2 2-D \rightleftharpoons 3-D