Identifying localized and delocalized electrons. Your ability to assign hybridizations to atoms with confidence and then to draw accurate 3D orbital pictures rests completely on being able to identify the delocalizable and localized electrons associated with the atoms in a molecular structure; so be sure you are clear and confident about identifying, predicting, and drawing resonance contributors (Section 2.1). This ability is a critical prerequisite skill.

Assigning hybridizations. As seen in Figure 0235, the number of localized electron pairs also defines exactly the hybridization of that atom. Four localized electron pairs (covalent bonds and localized nbe) define the sp^3 hybridization; three localized electron pairs define sp^2 hybridization; and two localized electron pairs define sp hybridization.

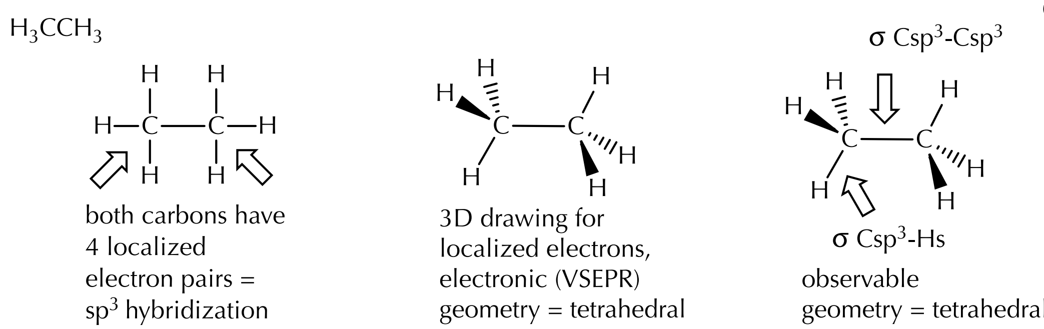
Drawing 3D orbital pictures. Once you have identified the hybridization, you can approach drawing a molecule in three stages. First: Draw the localized electron framework (see Figure 0230). Then, add in any unhybridized p orbitals that are needed on the sp^2 and sp atoms. Finally, add in the delocalizable electrons according to the resonance contributor that you are drawing. Up until the last step, the drawing is suitable for all resonance contributors.

Returning now to simple single, double, and triple bonding in hydrocarbons (see Figure 0225).

Ethane: H_3CCH_3 (Figure 0236). There are no delocalizable electrons (step 1). Both carbon atoms have 4 localized electron pairs, and so both are sp^3 hybridized (step 2). The electronic geometry for both carbons is tetrahedral, as is the observable geometry at both carbon atoms (step 3). There are 7 sigma (σ) bonds in the structure: 1 carbon-carbon sigma bond made from combining 2 sp^3 orbitals, and 6 carbon-hydrogen σ bonds made from combining a carbon sp^3 with a hydrogen s. The tetrahedral representation is used for both carbon atoms and the components of the bonds can be defined.

Figure 0236

Construction of a 3D orbital drawing for ethane (H_3CCH_3).



The other two hybridizations include 1 to 2 unhybridized p orbitals. An unhybridized p orbital can be empty (as in the case of an open shell atom), filled by a delocalizable electron pair, or it can be sharing electrons with another p orbital that is parallel to it, which is called pi (π) bonding.

Ethene: H_2CCH_2 (Figure 0237). Ethene has 1 delocalizable electron pair, because of the double bond, and 5 localized pairs. Both of the carbons have 3 localized electron pairs, and so both are sp^2 hybridized. The electronic geometry for both carbons is trigonal planar, as is the observable geometry at both carbons atoms. There are 5 sigma bonds in the structure: 1 carbon-carbon sigma bond made from combining 2 sp^2 orbitals, and 4 carbon-hydrogen sigma bonds made from combining a carbon sp^2 with a hydrogen s.

Each of the sp^2 carbon atoms carries an unhybridized p orbital, and there will be a pair of electrons shared (delocalized) between these two carbon atoms by the pi bonding overlap of those two p orbitals when they are parallel to one another.