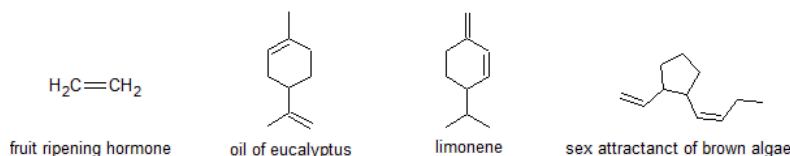


8.1: ALKENE STRUCTURE

Learning Objective

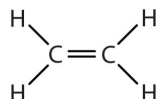
- describe the electronic structure of alkenes using Molecular Orbital (MO) Theory and Orbital Hybridization

Alkenes are a class of **hydrocarbons** (i.e., containing only carbon and hydrogen). They are unsaturated compounds with at least one carbon-to-carbon double bond. The double bond makes alkenes more reactive than alkanes. Olefin is another term used to describe alkenes. The alkene group can also be called a vinyl group and the carbons sharing the double bond can be called vinyl carbons.



ALKENES

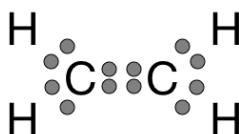
Nomenclature of alkenes is covered in chapter 3. Condensed structural formulas for the first eight alkenes are listed in Table 8.1.1 along with some relevant physical properties. Thus, $\text{CH}_2=\text{CH}_2$ stands for



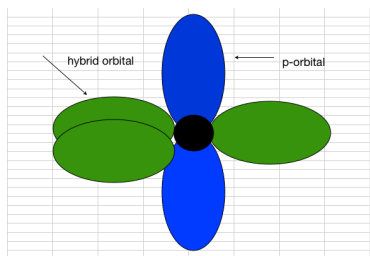
The double bond is shared by the two carbon atoms and does not involve the hydrogen atoms, although the condensed formula does not make this point obvious. Note that the molecular formula for ethene is C_2H_4 , whereas that for ethane is C_2H_6 .

STRUCTURE OF ETHENE - THE SIMPLEST ALKENE

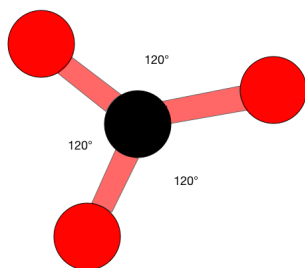
Ethene is not a very complicated molecule. It is made up of four $1s^1$ hydrogen atoms and two $2s^2 2p_x^1 2p_y^2$ carbon atoms. These carbon atoms already have four electrons, but they each want to get four more so that they have a full eight in the valence shell. Having eight valence electrons around carbon gives the atom itself the same electron configuration as neon, a noble gas. Carbon wants to have the same configuration as Neon because when it has eight valence electrons carbon is at its most stable, lowest energy state, it has all of the electrons that it wants, so it is no longer reactive.



This forms a total of three bonds to each carbon atom, giving them an sp^2 hybridization. Since the carbon atom is forming three sigma bonds instead of the four that it can, it only needs to hybridize three of its outer orbitals, instead of four. It does this by using the $2s$ electron and two of the $2p$ electrons, leaving the other unchanged. This new orbital is called an sp^2 hybrid because that's exactly what it is, it is made from one s orbital and two p orbitals.



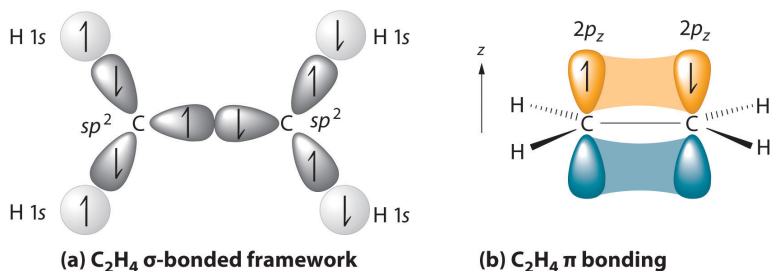
When atoms are an sp^2 hybrid they have a trigonal planar structure. These structures are very similar to a 'peace' sign, there is a central atom with three atoms around it, all on one plane. Trigonal planar molecules have an ideal bond angle of 120° on each side.



The H-C-H bond angle is 117° , which is very close to the ideal 120° of a carbon with sp^2 hybridization. The other two angles (H-C=C) are both 121.5° .

RIGIDITY IN ETHENE

There is rigidity in the ethene molecule due to the double-bonded carbons. A double bond consists of one sigma bond formed by overlap of sp^2 hybrid orbitals and one pi bond formed by overlap of parallel 2 p orbitals. In ethene there is no free rotation about the carbon-carbon sigma bond because these two carbons also share a π bond. A π bond is only formed when there is adequate overlap between both top and bottom p-orbitals. Free rotation the p-orbitals cause them to be 90° from each other breaking the π bond because there would be no overlap. Since the π bond is essential to the structure of ethene it must not break, so there can be no free rotation about the carbon-carbon sigma bond. The two carbon atoms of a double bond and the four atoms attached to them lie in a plane, with bond angles of approximately 120° as shown in the figure below



(a) The σ -bonded framework is formed by the overlap of two sets of singly occupied carbon sp^2 hybrid orbitals and four singly occupied hydrogen $1s$ orbitals to form electron-pair bonds. This uses 10 of the 12 valence electrons to form a total of five σ bonds (four C-H bonds and one C-C bond).

(b) One singly occupied unhybridized $2p_z$ orbital remains on each carbon atom to form a carbon-carbon π bond. (Note: by convention, in planar molecules the axis perpendicular to the molecular plane is the z-axis.)

The first two alkenes in Table 8.1.1, ethene and propene, are most often called by their common names—ethylene and propylene, respectively (Figure 8.1.1). Ethylene is a major commercial chemical. The US chemical industry produces about 25 billion kilograms of ethylene annually, more than any other synthetic organic chemical. More than half of this ethylene goes into the manufacture of polyethylene, one of the most familiar plastics. Propylene is also an important industrial chemical. It is converted to plastics, isopropyl alcohol, and a variety of other products.

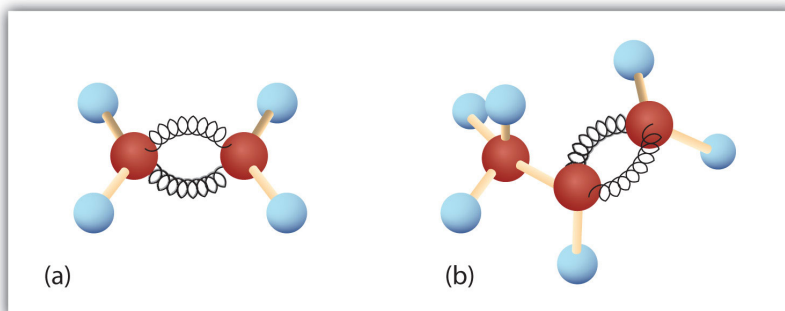


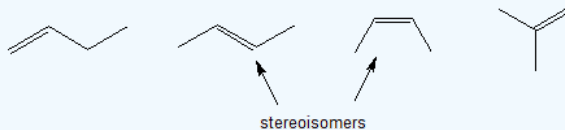
Figure 8.1.1: Ethene and Propene. The ball-and-spring models of ethene/ethylene (a) and propene/propylene (b) show their respective shapes, especially bond angles.

Exercise

1. Although there is only one alkene with the formula C_2H_4 (ethene) and only one with the formula C_3H_6 (propene), there are several alkenes with the formula C_4H_8 . Draw all of the possible bond line structures for alkenes with the formula C_4H_8 including all possible structural and stereoisomers.

Answer

1. There are three possible structural isomers. 2-butene can exist as two different stereoisomers.



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