5.111 Principles of Chemical Science: Week 5

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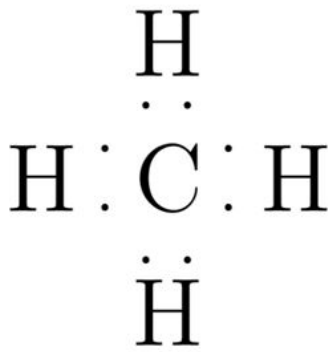
Progress Update

Over the past week I have been introduced to:

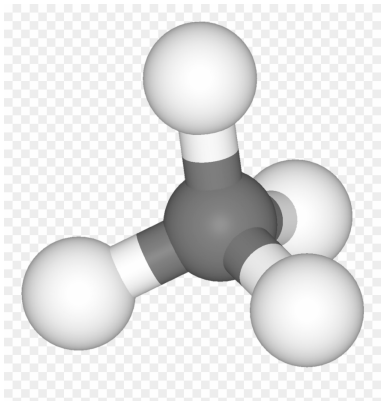
1. VSEPR theory.
2. Molecular orbital theory.
3. Orbital hybridization.

VSEPR Theory

The basis of the VSEPR theory is that the electrons and bonds in a molecule wish to minimize repulsion. Consider the Lewis structure of methane:

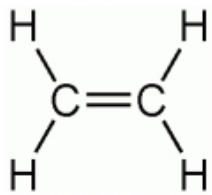


In order to minimize the repulsion caused by these bonds being near eachother, the molecule takes on a tetrahedral shape:

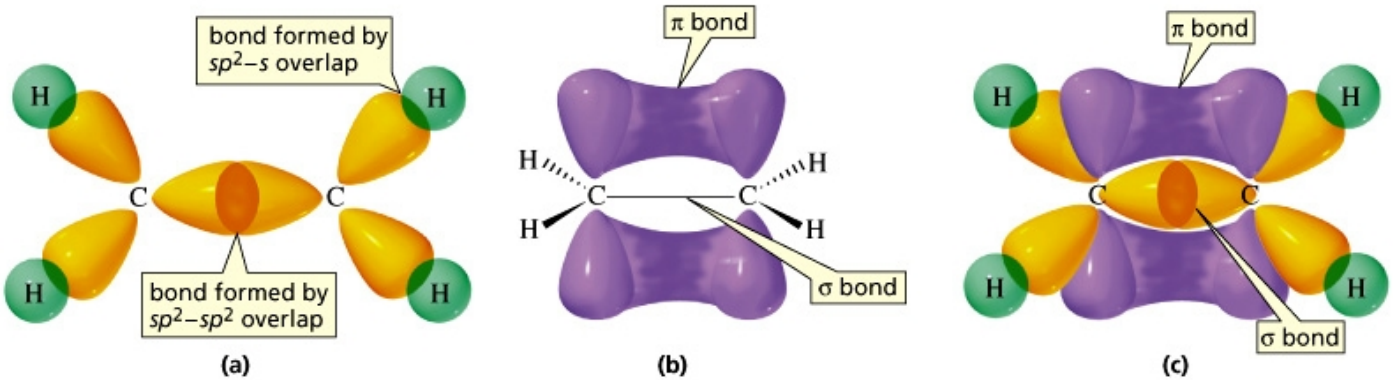


Molecular orbital theory

Molecular orbital theory states that the bonds in a molecule result from constructive and destructive interference between the 2 atoms orbitals. 2 kinds of orbitals exist: σ (sigma) and π (pi). Consider the bonds in ethylene:

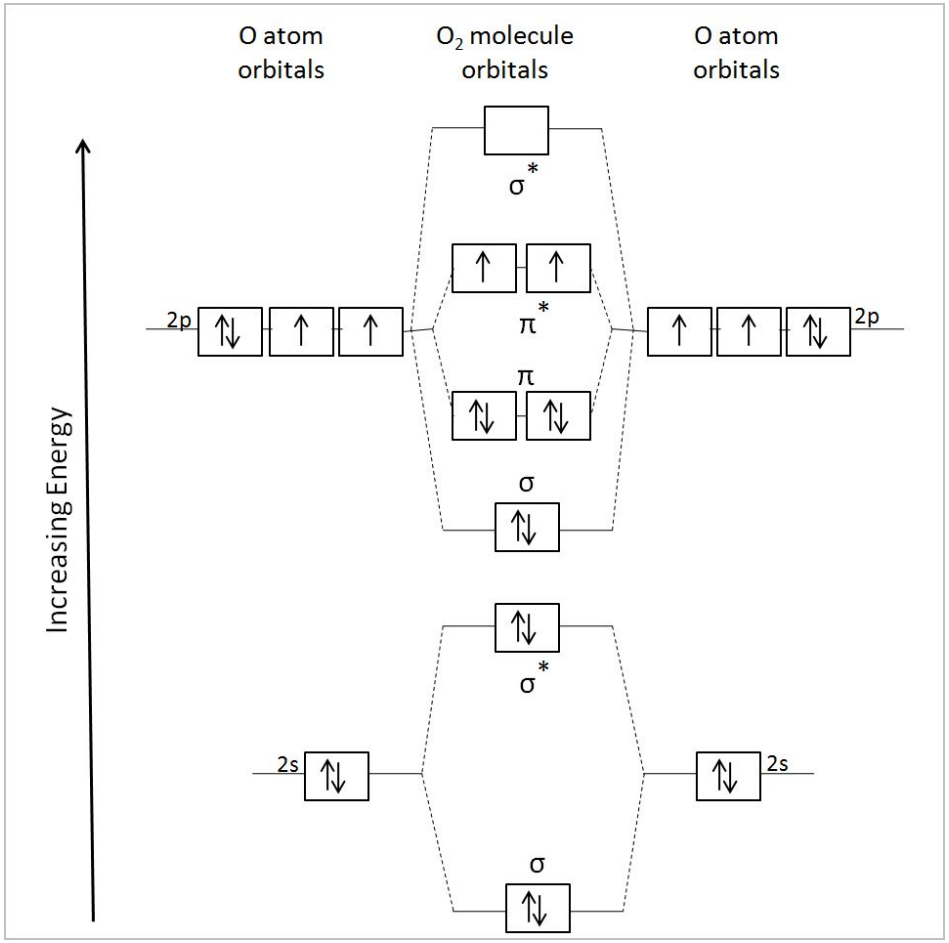


Ethylene (Ethene)



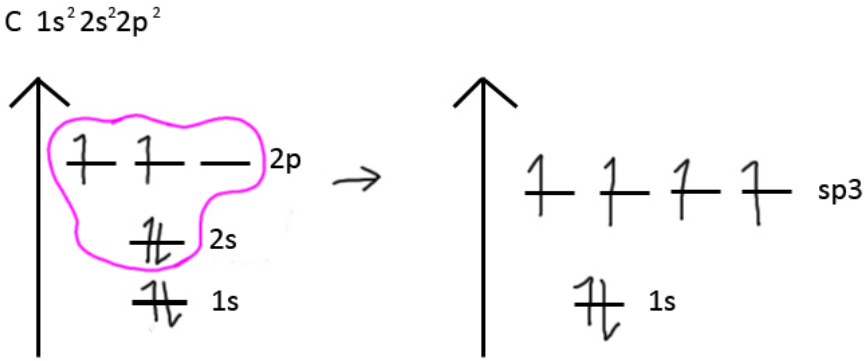
Molecular orbital theory (continued)

Consider the *molecular orbital diagram* of O_2:



Orbital hybridization

Orbital hybridization is the technique of mixing orbitals and moving electrons to allow for more bonds to be made:



First an electron is moved from an s orbital to a p orbital, then the s orbital mixes with the p orbitals to produce orbitals of lower (and thus more rewarding to pair) energy.

Olympiad problem

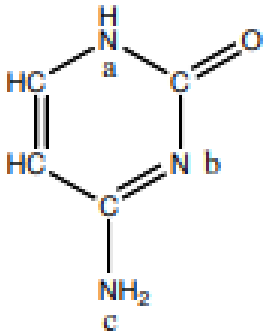
Problem: Which statement about bonding is correct?

1. (A) A σ bond has cylindrical symmetry about the bonding axis.
2. (B) A π bond is twice as strong as a σ bond.
3. (C) A double bond consists of two π bonds.
4. (D) A π bond results from the sideways overlap of hybridized orbitals.

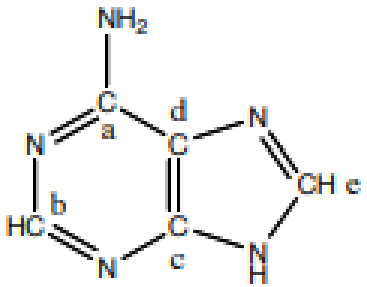
Lecture problem

Consider the problem

For the DNA bases below, assign the **hybridization** and **geometry** to
(a) the nitrogen atoms in cytosine, and
(b) the carbon atoms in adenine. (Note that the lone pairs are not pictured.)



cytosine



adenine

(a) N_a: sp^3, trigonal pyramidal, N_b: sp^2, bent, N_c :sp^3, trigonal pyramidal
(b) All of the carbon atoms are sp^2, trigonal planar.