Chem 4A Scolars Notes

Drawing MO Diagrams for Polyatomic Molecules

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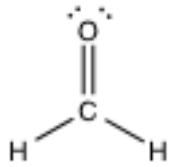
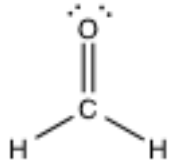
Drawing molecular orbital(MO) diagrams for polyatomic orbitals can be divided into three steps. Here we will use CH_2O as an example.

1. Determine the lewis stucture of the molecule.



2. Use VSEPR to decide the electronic and molecular geometry of the molecule.

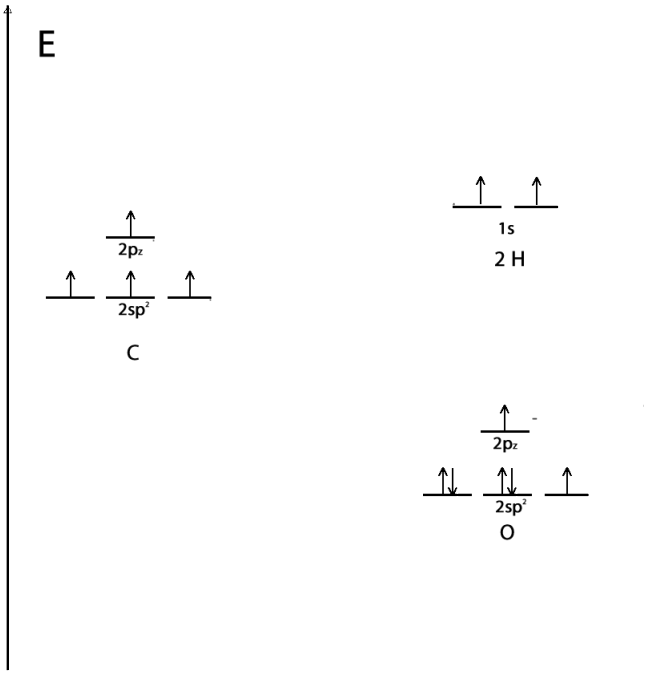
   CH_2O is trigonal plannar.



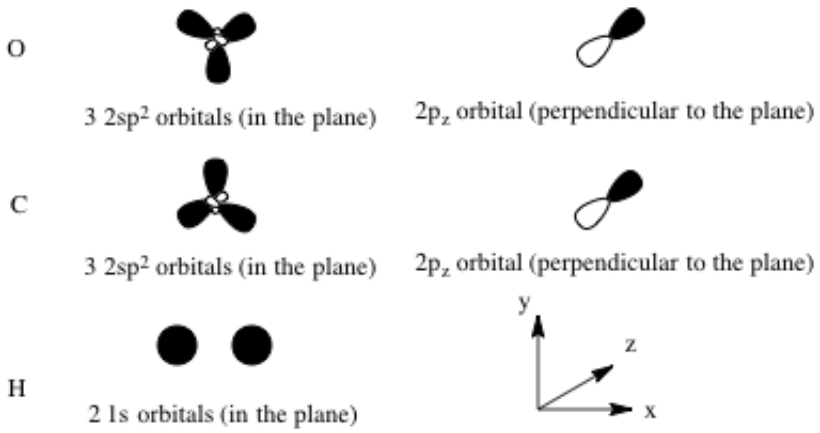
3. Basing on the geometry, choose the right hybridization for the atoms.

   The carbon atom is sp^2 hybridized. Oxygen atom has 2 lone pairs and is also sp^2 hybridized.

4. For each atom, prepare their hybridized atomic orbitals(HAOs) from their valence atomic orbitals(VAOs). and fill electrons in them.

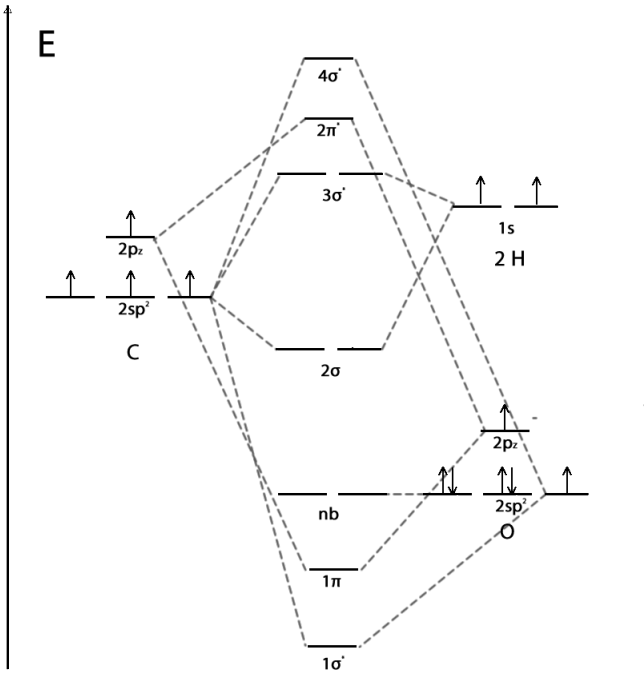


5. By observing the geometry of the molecule and symmetry of the orbitals, decide which pairs orbitals interact.

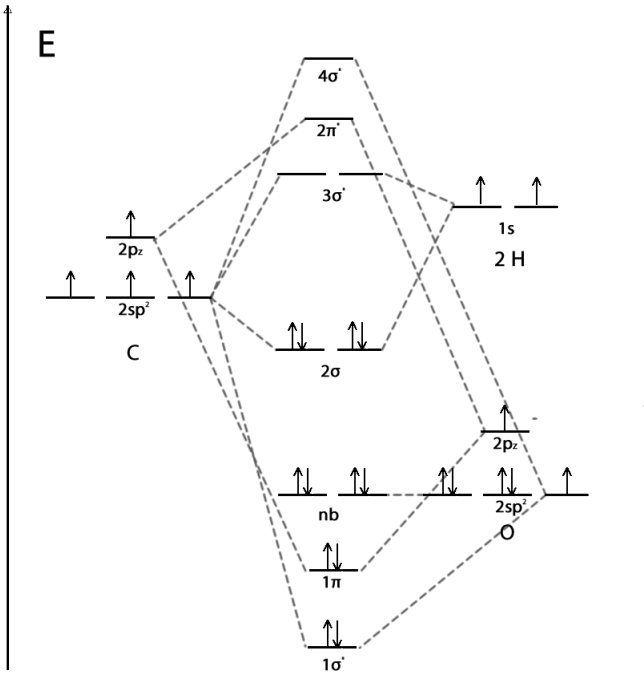


From here we can tell that sp^2 orbitals of carbon will form three σ- bond with the 1s orbitals of the hydrogen atoms and one of the sp^2 orbital of the oxygen atom. There is a π-bond between the two p_z orbitals.

6. For each pair of the interacting AOs, create an bonding and anti-bonding orbital(*), give them the right label and energy. Non-interacting AOs are marked as non-bonding orbitals, usually noted as nb. Lone pairs can also be noted as lp. σ orbitals and π orbitals' label number starts from 1 and increase independently as the energy level goes up.



7. Fill the electrons into the MOs from lowest to highest energy. Remeber you should still follow Hund's rule in make MO diagrams.



8. If asked, calculate the bond order.

   Bonder order = (bonding electrons - antibonding electrons) / 2

   Here,

   Bonder order = (8 - 0) / 2 = 4

9. Congratulations, you've made a MO diagram!