MO Diagrams for Linear Triatomic Molecules

Skills to Develop

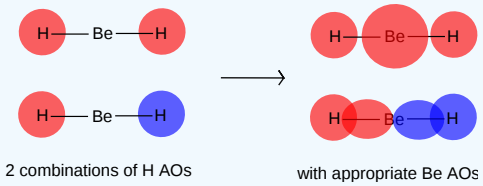
- Construct MO diagrams for simple linear triatomic molecules and/or compounds

What's Different if we have 3 Atoms?

We won't go into the details of MO theory for complex molecules, because that's a topic for more advanced classes, like Inorganic Chemistry. However, we'll show a couple examples of simple molecules so you can get the idea. We'll focus on molecules with 1 central atom and some others around it. In this case, first we combine the AOs of the outer atoms into sensible combinations, then we see how these combinations interact with the AOs on the central atom. Don't forget about **net overlap**, which is important for deciding how the orbitals interact. If they don't have net overlap, they can't interact.

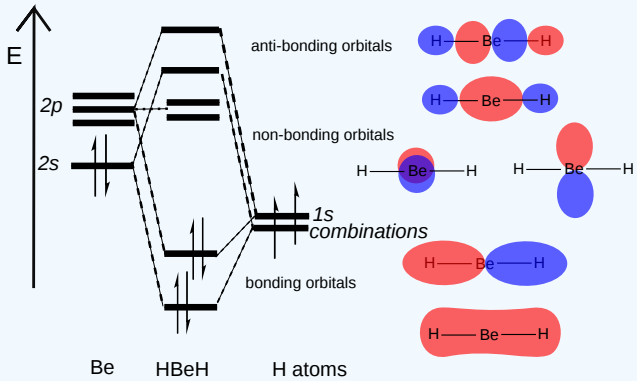
2

BeH_2 might be hard to make, but it's very nice and simple as an example! Using the electron domain model we predict that it will be linear. Be has 2s and 2p orbitals, and it is in the middle. H has 1s orbitals; there are 2 H atoms on the outside. We need to make combinations of the H AOs, and we'll use the same combinations we used to make H_2, except now they aren't touching. These combinations will match the 2s and $2p_z$ on Be, as shown in the figure.



Forming MOs for BeH_2.

Then we can put the MO diagram together just the way we usually do, starting with the outside, drawing in bonding, non-bonding and anti-bonding MOs, and filling the electrons. The bond order is 2.



MO diagram for BeH_2.

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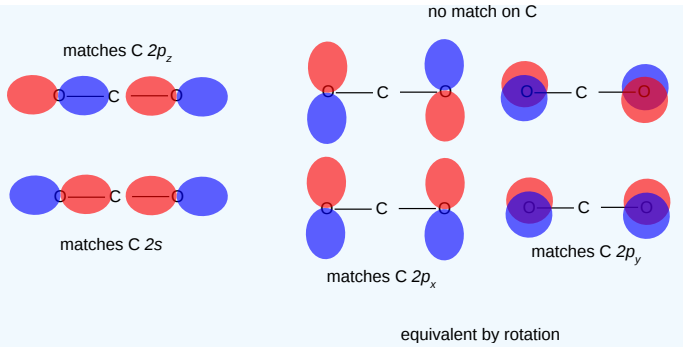
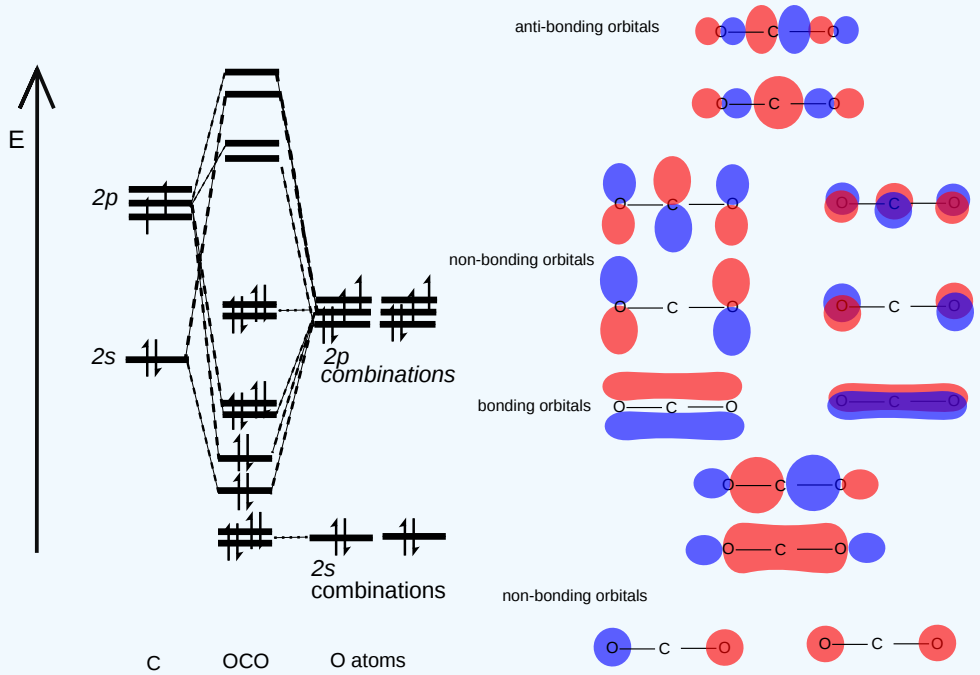
This is a little more complicated example. Now we have to make combinations of 4 different AOs from oxygen. We can combine 2s orbitals, $2p_x$ orbitals, $2p_y$ orbitals and $2p_z$ orbitals. Each pair will make the same add/subtract combinations we've seen before. However, for a basic diagram, we will include only the O 2p orbitals, because the O 2s orbitals are much lower in energy; they have a bad energy match so they won't interact very much. The O 2p combinations that we will use are shown in the figure, and labeled with which carbon AO they match.



Oxygen AO combinations for CO_2.

Then we combine these oxygen AO combinations with the AOs on C. We still make bonding and anti-bonding combinations just like before. And there are some non-bonding orbitals too. Just as we expect from Lewis structures, there are 2 σ bonds and 2 π bonds. However, each of these is **delocalized** over the whole molecule. The bonds aren't just between 2 atoms at a time, they connect all 3 atoms.



MO diagram for CO_2.

Contributors and Attributions

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