MO Diagrams for Heterodiatomic Molecules

Skills to Develop

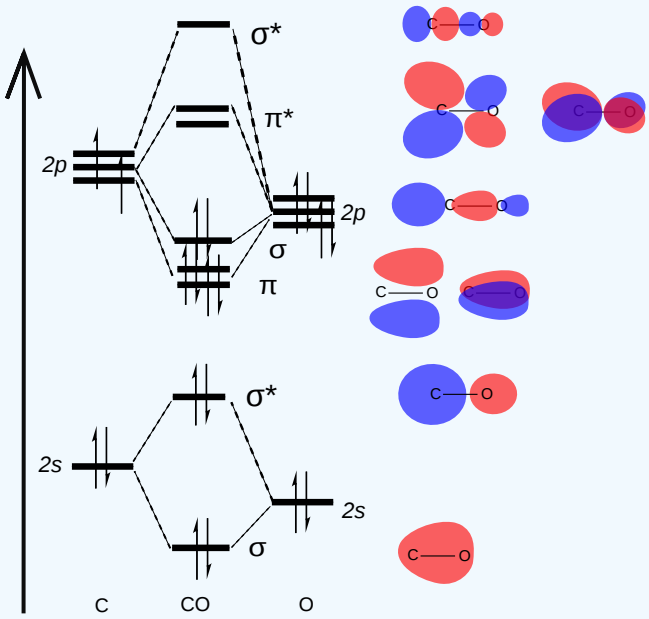
- Construct MO diagrams for simple diatomic compounds

What's Different if we have 2 Elements?

If the elements are different, the main thing is that the AOs won't have the same initial energy. If they don't have the same energy, then the splitting will be smaller. Also, the bonding MO will have a higher % of the lower energy AO and the anti-bonding MO will have a higher % of the higher energy MO. This is exactly the same as saying that it will make a polar covalent bond. The electrons will usually be in the bonding MO, not the anti-bonding MO. The bonding MO has more of the lower energy AO, so the electrons will spend more time next to the atom with lower AOs, which is the same as the more electronegative atom. The bigger the difference in electronegativity/AO energy, the smaller the splitting and the more the bonding MO looks like the AO of the electronegative atom. When the difference is really big, the bond becomes completely ionic, and the "bonding MO" basically is the lower energy AO.

Example 1: CO

This diagram is based on calculations and comparison to experiments. (But it is not drawn exactly, just approximately.) It would be hard to guess all the details, especially about the sp-mixing and the shapes and sizes of MOs. Notice that the bonding orbitals are bigger on the oxygen and the antibonding orbitals are bigger on the carbon. We will talk more about the consequences of this later.



MO diagram for CO.

Contributors and Attributions

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