MO Diagrams for Water and Nitrate Ion

Skills to Develop

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

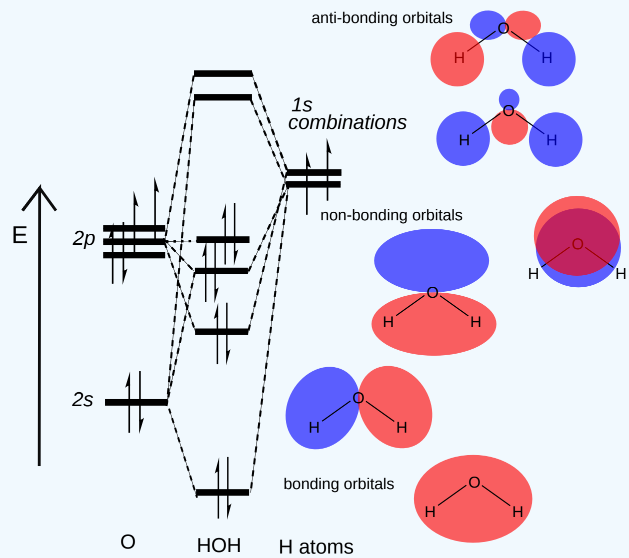
Non-linear Molecules

If you take an Inorganic Chemistry class, you'll learn ways to make MO diagrams for more complicated, non-linear molecules. Here we won't really explain these methods, just show some results. First we'll look at an MO diagram for water, because it's pretty simple and water is very important. Then we'll look at the π MOs for the nitrate ion, so we can see the difference between MO theory and valence bond theory.

Example 1: Water

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 hydrogen. This produces the polarity that makes water a good solvent, because there is more electron density on the O and less electron density on the H.

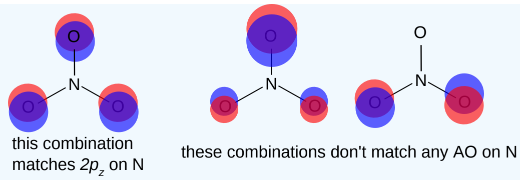
We start by making the same H AO combinations we used for H_2 and also for BeH_2. Then we do sp-mixing on O, making one orbital pointed toward the H atoms and one pointed away (which will be mostly non-bonding, like a lone pair). Then we make bonding and anti-bonding combinations of H and O orbitals that match.



MO diagram for water.

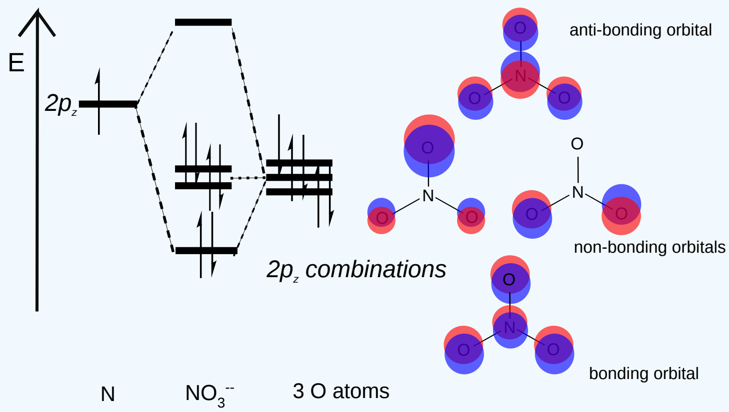
Example 2: Nitrate ion π MOs

In the section on multiple bonds using Valence Bond Theory, we talked about nitrate ion (NO_3^-), which has 1 π bond shared over 4 atoms (3 different resonance structures). That might have seemed kind of weird, so let's look at it again using MO theory, which treats resonance much more naturally. Let's just think about the 4 $2p_z$ orbitals, on 1 N and 3 O atoms. These orbitals point out of the plane of the molecule and will be used to make π bonds. First we will make combinations of the oxygen AOs. The combinations are shown in the figure. Don't worry about where these combinations came from too much, because that's a little too advanced for us (you'll see, if you take an Inorganic Chemistry class).



Oxygen π AO combinations for nitrate ion.

You can see that 2 of the combinations don't match the AOs on N, so they will be non-bonding MOs (like 2 lone pairs shared over 3 O atoms). One combination matches the N orbital, so it will make bonding and anti-bonding combinations. There are 6 π electrons in nitrate, so the bonding and non-bonding MOs will be filled. This means there is one π bond shared over the 4 atoms, which is just what valence bond theory says also.



π MO diagram for nitrate ion.

Contributors and Attributions

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