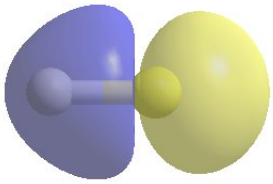
Answers to Exercise 3.1
Linear Combination of Atomic Orbitals: Heteronuclear Diatomics

1. *The white atom on the left is H. The yellow atom on the right is F.*

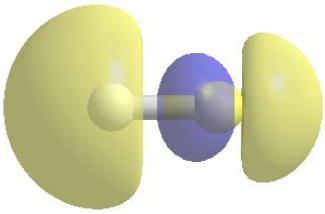
(a)



This is a sigma bonding molecular orbital.

Your picture should look like it has a larger contribution from the 2p orbital on F and a smaller contribution from the 2s orbital on H. In other words, like a "big" 2p on F combined with a "small" 2s on H. This is because this MO is closer in energy to the lower energy AO from which it was formed (the 2p orbital on F).

(b)

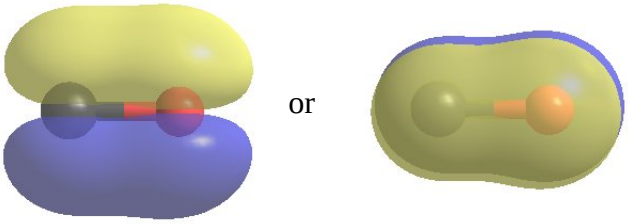


This is a sigma antibonding molecular orbital.

Your picture should look like it has a large contribution from the 2s orbital on H and a small contribution from the 2p orbital on F. In other words, like a "big" 2s on H combined with a "small" 2p on F. This is because this MO is closer in energy to the higher energy AO from which it was formed (the 2s orbital on H).

2. *The black atom on the left is C. The red atom on the right is O.*

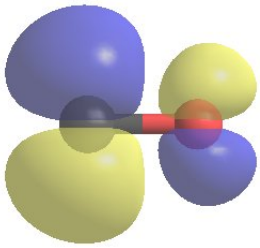
(a)



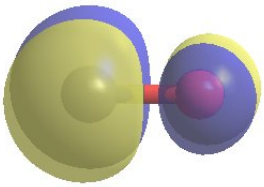
This is a pi bonding molecular orbital.

Your picture should look like it has a larger contribution from the 2p orbital on O and a smaller contribution from the 2p orbital on C. In other words, like a "big" 2p on O combined with a "small" 2p on C. This is because this MO is closer in energy to the lower energy AO from which it was formed (the 2p orbital on O). (This is easier to see on the picture on the right than the one on the left. When drawing by hand, it's fine to exaggerate the difference.)

(b)



or



This is a pi antibonding molecular orbital.

Your picture should look like it has a larger contribution from the 2p orbital on C and a smaller contribution from the 2p orbital on O. In other words, like a "big" 2p on C combined with a "small" 2p on O. This is because this MO is closer in energy to the lower energy AO from which it was formed (the 2p orbital on C).

3. most polarization to least polarization: $CO > CN^- > N_2$

The amount of polarization increases as the difference in energy between the atomic orbitals being combined increases. Elements with larger ionization energy have valence atomic orbitals with lower energy. As such, we can expect the $2p$ orbitals of O to be lower in energy than the $2p$ orbitals of N which will, in turn, be lower in energy than the $2p$ orbitals of C. Thus:

- there will be no polarization of the π MOs in N_2 since both $2p(N)$ have the same energy.
- there will be some polarization of the π MOs in CN^- since $2p(N)$ has slightly lower energy than $2p(C)$.
- there will be more polarization of the π MOs in CO since the energy gap between $2p(O)$ and $2p(C)$ is larger than the energy gap between $2p(N)$ and $2p(C)$.

Some people prefer to talk about electronegativity instead of ionization energy when discussing the degree of polarization in MOs. Since the two trends are the same for most elements, that usually works; however, it can lead to problems if discussing a molecule containing a noble gas.