## Diatomics of the Second Row

In the same way as we think about $H_2$ we can think about diatomics of the second row. Commonly these are things such as $O_2$ and $N_2$, but for ease of thinking about it we'll work from $Li_2$ right the way across to $F_2$. We need to start off by thinking about which of the orbitals will interact significantly. Here we find that the full 1s-orbitals are significantly smaller than the 2s-orbitals. This means that there is very little interaction between the 1s-orbitals, so we can concentrate on the 2s and 2p interactions.

Starting off with the 2s-orbitals: these are the same shape as the 1s-orbitals and therefore the way that two 2s-orbitals interact is the same as the 1s-orbitals above, giving us one bonding and one anti-bonding molecular orbital. Then we have to consider the 2p-orbitals; here things get a little more complicated as these can interact in different ways: forming either sigma – through the overlap of one lobe - or pi – through the overlap of two lobes - interactions. These are both shown in Figure 1.

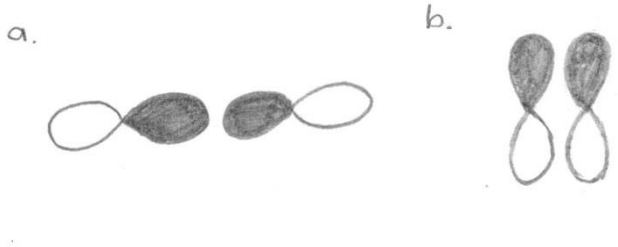


Figure 1. Showing the sigma, σ, and pi, π, interactions possible from two p-orbitals. In a) we have a sigma interaction from the overlap of one lobe, in b) two lobes interact giving a pi orbital.

These sigma and pi interactions are of different strength, with the sigma bonding interaction being more favourable, giving more additional stability, than the pi interaction and vice versa the anti-bonding sigma interaction being more destabilising than the pi one. This gives us the MO diagram showed in Figure 2a. Now we can think about putting in the electrons for the first of our diatomics, $O_2$. In this case we are going to ignore the 1s electrons and just concentrate on those in the 2$^{nd}$ shell, the outcome is shown in Figure 2b.

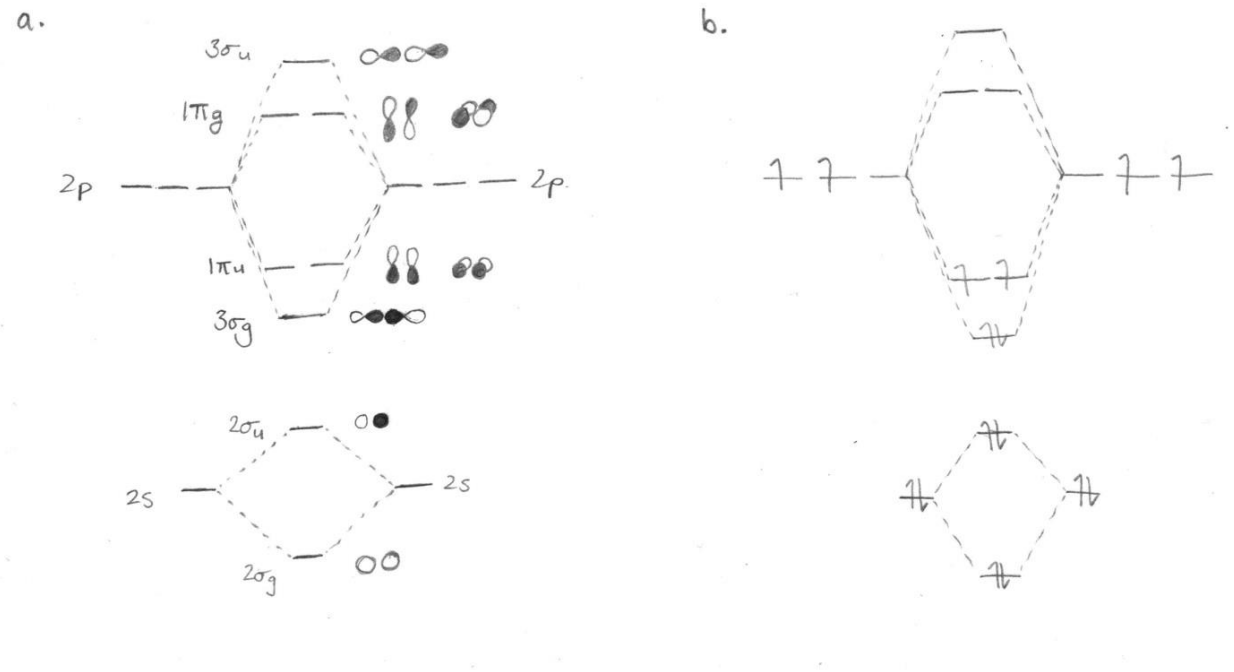


Figure 2. a) showing how the molecular orbital diagram from the interaction of two 2s and 2p orbitals and b) the same diagram with the electrons for $O_2$ present (the orbital labels used here are composed e.g. $2\sigma_u$ with the 2 showing us this is the second orbital of this type (the first would have been made from the 1s orbitals which isn't shown in this diagram; the σ tells us the type of overlap we have and the u is a symmetry label. For this final letter a $_u$ means that the phase changes as we pass through the centre of inversion whereas a $_g$ means the phase stays the same.

Question: Can you work out the bond order for $O_2$ and draw the MO diagram for $F_2$, what is the bond order here?