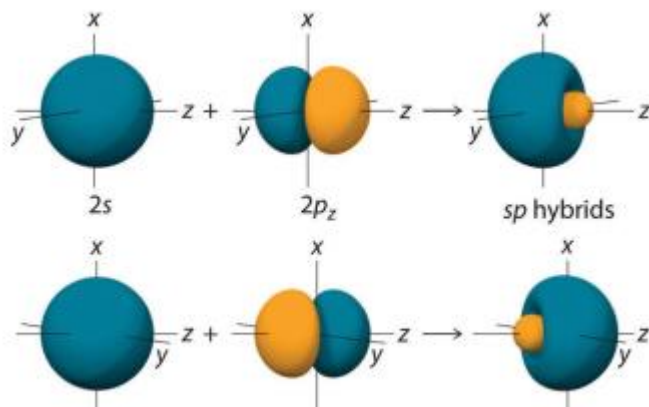
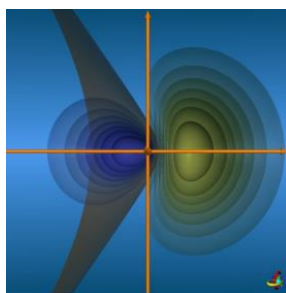
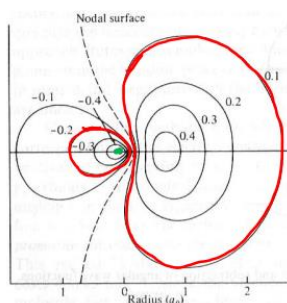
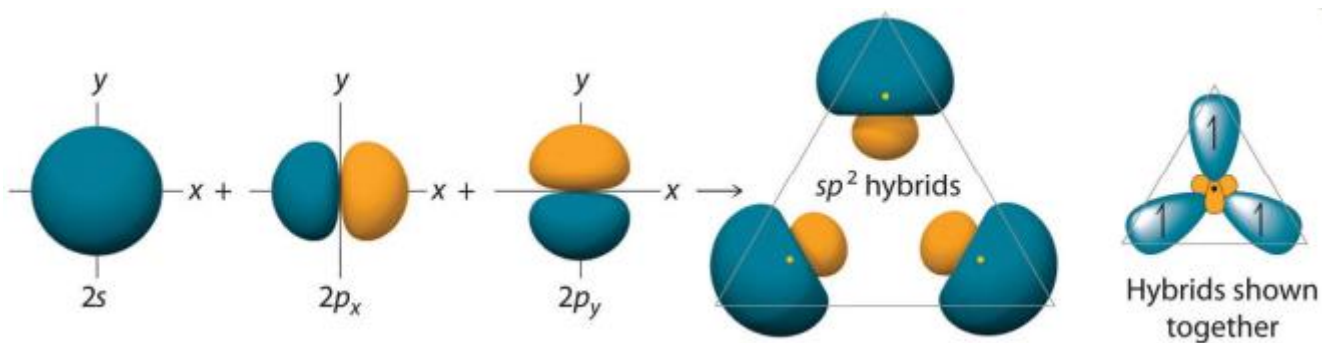


1. sp Hybrid Orbitals

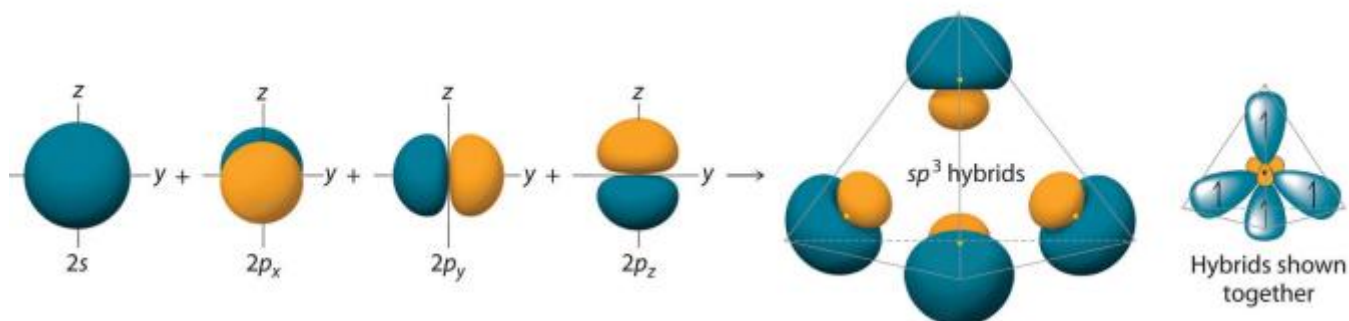


Make sure the nucleus is not on the nodal surface.
Indicate the signs as well in your sketches.

sp^2 Hybrid Orbitals



sp^3 Hybrid Orbitals

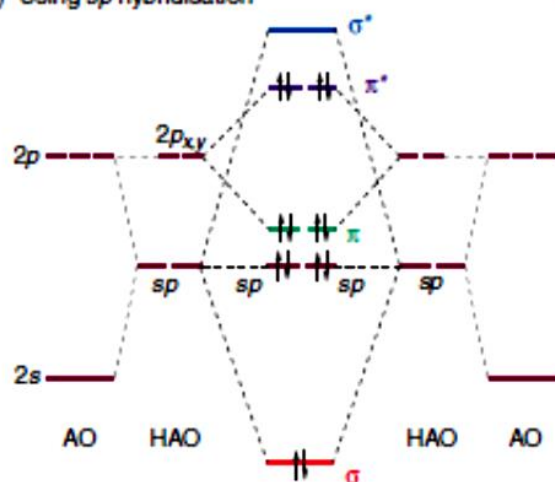


2. If we use sp HAOs on the F atoms, we can describe the bonding by saying that two sp HAOs (one on each atom) overlap to produce a σ bonding MO and a σ^* antibonding MO; the σ MO is filled. The remaining sp HAO on each atom points outward and is occupied by two electrons to give a lone pair. The unhybridised p orbitals on each F atom can overlap to form a pair of π bonding MOs and a pair of π^* antibonding MOs. The total number of electrons is 14, and these occupy the σ MO, the two sp lone pairs and all of the π and π^* MOs.

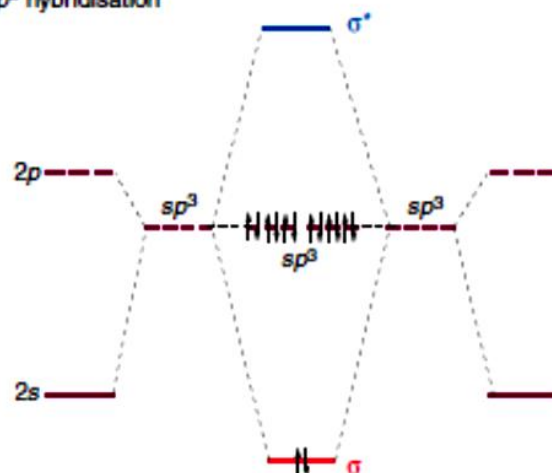
If instead we assume that the F atoms are sp^3 hybridised, we can describe the bonding in terms of overlap of two sp^3 HAOs (one from each atom) generating a σ bonding MO and a σ^* antibonding MO. Occupation of the bonding MO by two electrons produces an F-F σ bond. The remaining six sp^3 HAOs (three on each atom), which we will assume do not interact with each other since they are pointing outward, or at least not pointing directly at the other atom, accommodate two electrons each to give six lone pairs.

The resulting MO diagrams are shown below, together with that from the full MO approach (from Fig. 4.27 on page 122).

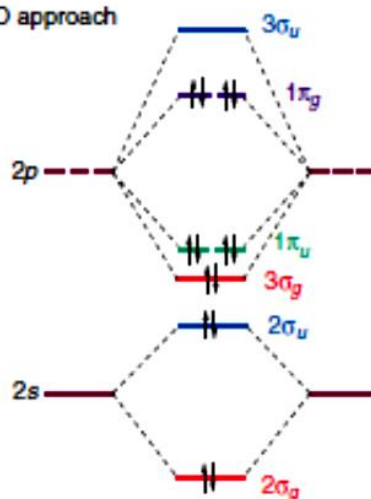
(i) Using sp hybridisation



(ii) Using sp^3 hybridisation



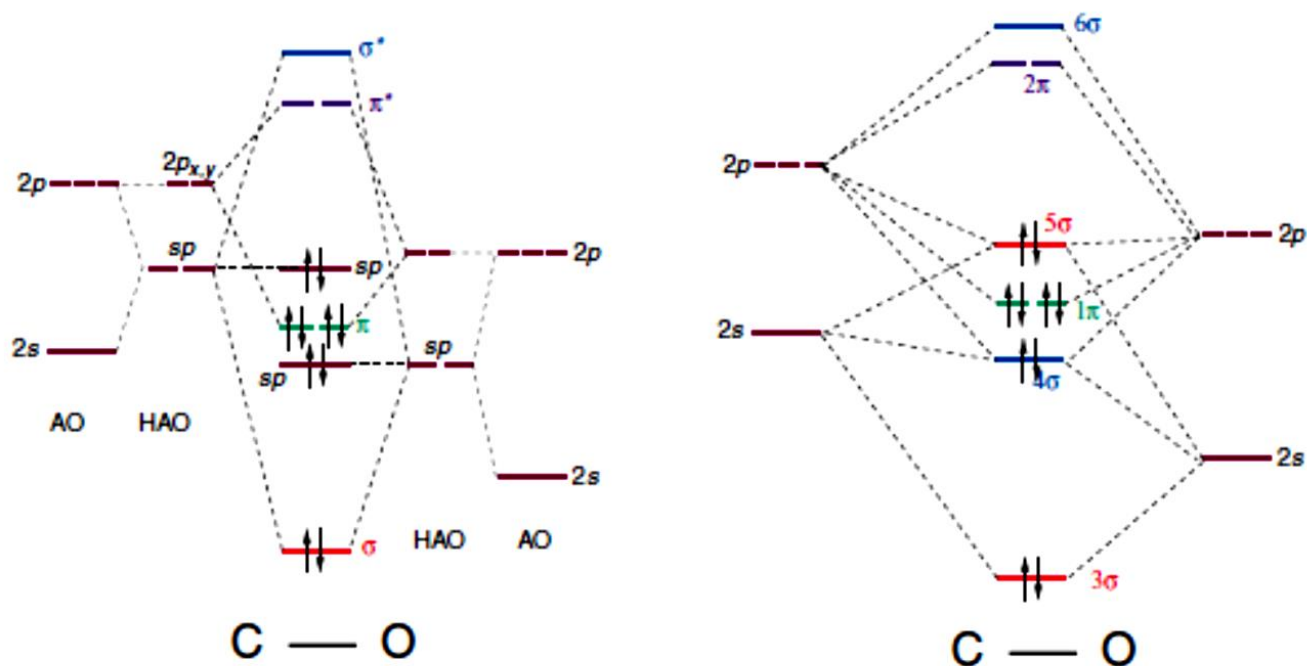
Full MO approach



There are some similarities between the diagrams. Using sp HAOs, we have a low lying σ MO (corresponding to $2\sigma_g$) which we interpret as giving rise to a σ bond. We also have filled π and π^* orbitals, just as in the full MO treatment. However, use of sp hybrids predicts two nonbonding lone pairs rather than a weakly antibonding MO ($2\sigma_u$) and a weakly antibonding MO ($3\sigma_g$).

3. The MO diagrams for CO is shown here. For NO, it will be similar, only the HOMO will be a singly filled π^* (i.e., just one more electron will be present in case of NO (11 e⁻) than CO (10 e⁻)).

Using a similar approach for CO, assuming sp hybridisation for both atoms, we obtain the following MO diagram. For comparison, the MO diagram from Fig. 4.40 on page 136 is also shown.



The overall form of the two diagrams is remarkably similar: both predict one σ bond (corresponding to the bonding MO labelled 3σ in the diagram on the right) and two π bonds.

The hybrid approach gives two nonbonding orbitals (one sp HAO on C and one on O) while the full MO picture gives two orbitals (labelled 4σ and 5σ) which are neither strongly bonding nor antibonding.

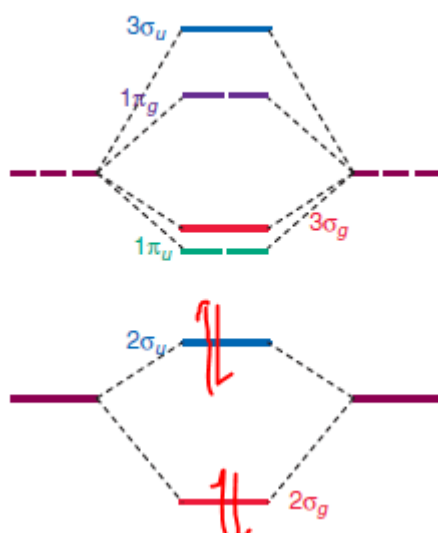
The hybrid approach gives the HOMO as the sp HAO on carbon. The full MO approach gives the HOMO as the 5σ MO, which does indeed have its largest contribution from the carbon (as shown below), but also has a significant contribution from the oxygen which is not predicted by the hybrid approach.



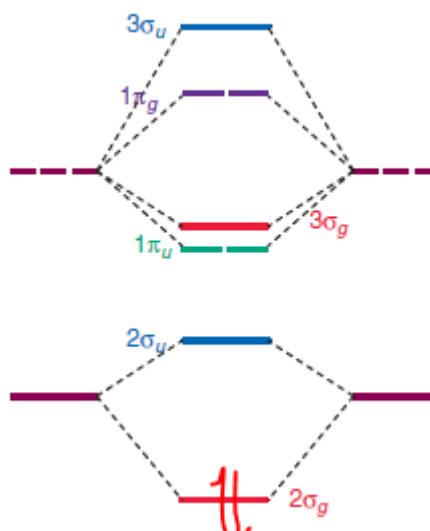
Both approaches give the LUMO as the C–O π^* antibonding MO (labelled 2π in the diagram for the full MO approach).

4.

Be₂ MO Diagram



Li₂ MO Diagram



- a) In case of Be₂, **bond order = 0** (occupation of bonding and antibonding MOs result in no net bonding)

However, the effect of the *s-p* mixing is that (i) the bonding $2\sigma_g$ MO is lowered in energy (i.e. it becomes *more bonding*), and (ii) the antibonding $2\sigma_u$ MO is also lowered in energy (i.e. it becomes *less antibonding*). As a result, the bonding and antibonding effects of these two MOs do not cancel one another out, leading to net bonding overall, albeit rather weak.

- (b) There are two valence electrons in Li₂, which occupy the bonding $2\sigma_g$ MO. In contrast to Be₂, Li₂ simply has bonding electrons, and this accounts for its much greater bond strength.