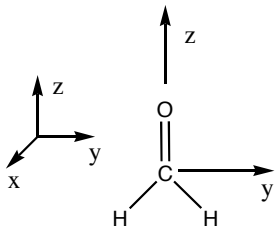
Construct the valence molecular orbital diagram for the formaldehyde H_2CO molecule oreintated as shown below. The O 2sAO does not remain non-bonding. A small amount of mixing occurs between the close lying occupied a_1 MOs.

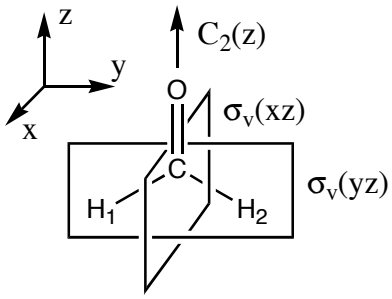


- Forming a MO diagram

1. determine the molecular shape and identify the point group of the molecule
2. define the axial system find all of the symmetry operations on the molecule
3. identify the chemical fragments, and put them along the bottom of the diagram
4. determine the energy levels and symmetry labels of the fragment orbitals
5. combine fragment orbitals of the same symmetry, estimate the splitting energy and draw in the MO energy levels and MOs (in pencil!)
6. determine the number of electrons in each fragment and hence the central MO region, add them to the diagram
7. identify if any MO mixing occurs, determine the mixed orbitals and redraw the MO diagram with shifted energy levels and the mixed MOs
8. use the MO diagram check-list!
9. analyse the MO diagram

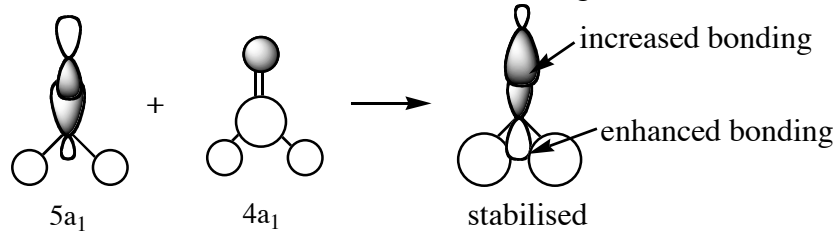
shape has been given, point group is C_{2v}

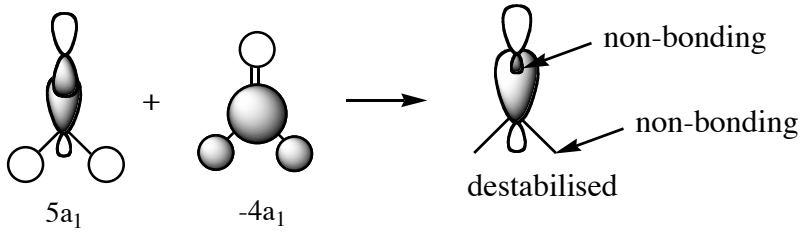
axial system has been defined, symmetry operations

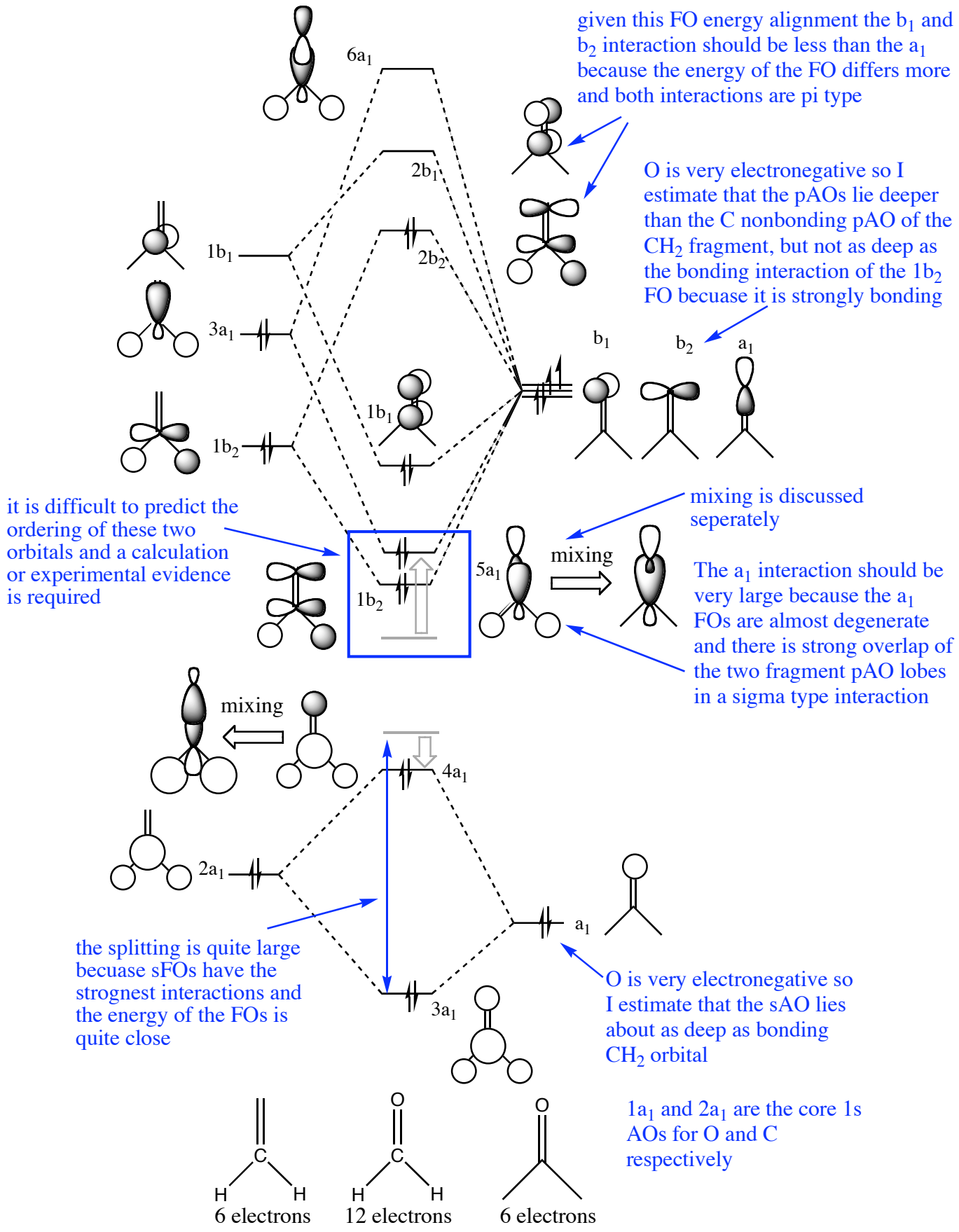


The MO diagram is shown over page

Mixing: MO mixing is unlikely to be large between occupied orbitals, because the antibonding MO will be destabilised by more than the bonding MO is stabilised, however the final arbeiter of mixing is the stability of the molecule as a whole, which must be the case here. The unoccupied $6a_1$ MO is very high in energy and thus too far away in energy from the occupied $4a_1$ MO for significant mixing to occur. We are told mixing occurs between the close lying occupied a_1 MOs, this must be the $4a_1$ and $5a_1$ MOs, mixing is depicted below and it will raise the energy of the $5a_1$ MO which becomes more non-bonding and lower the energy of the $4a_1$ MO which becomes more bonding as shown.







given this FO energy alignment the b_1 and b_2 interaction should be less than the a_1 because the energy of the FO differs more and both interactions are pi type

O is very electronegative so I estimate that the pAOs lie deeper than the C nonbonding pAO of the CH_2 fragment, but not as deep as the bonding interaction of the $1b_2$ FO becuase it is strongly bonding

it is difficult to predict the ordering of these two orbitals and a calculation or experimental evidence is required

mixing is discussed seperately

The a_1 interaction should be very large because the a_1 FOs are almost degenerate and there is strong overlap of the two fragment pAO lobes in a sigma type interaction

the splitting is quite large becuase sFOs have the strognest interactions and the energy of the FOs is quite close

O is very electronegative so I estimate that the sAO lies about as deep as bonding CH_2 orbital

$1a_1$ and $2a_1$ are the core 1s AOs for O and C respectively