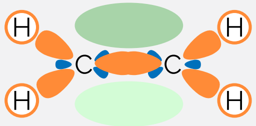
Valence bond theory & hybrid atomic orbitals

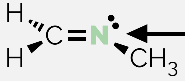
1. Introduction



Valence bond theory provides another representation of a molecule. In organic chemistry, it marries the simplicity of line diagrams to the accuracy of molecular orbital theory.

It is a useful compromise that allows the construction of orbital representations without computers.

2. Hybridisation



nitrogen
2 atoms + 1 lone pair
= 3 = sp^2

The hybridisation of an atom is given by:

#atoms attached + #lone pairs

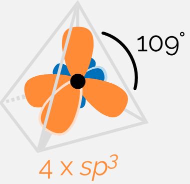
The total will be between 4 & 2:

4 = sp^3; 3 = sp^2; 2 = sp

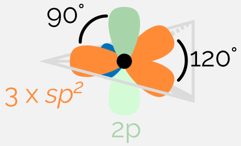
If an atom has a lone pair of electrons & it is adjacent to a π bond it will be sp^2.

These rules are a simplification!

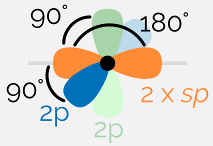
3. Hybrid atomic orbitals (HAO)



***sp³* hybrid**
Four HAOs made from the *2s* & 3 x *2p*. The *sp³* HAOs point to the corners of a tetrahedron with separation of 109˚.

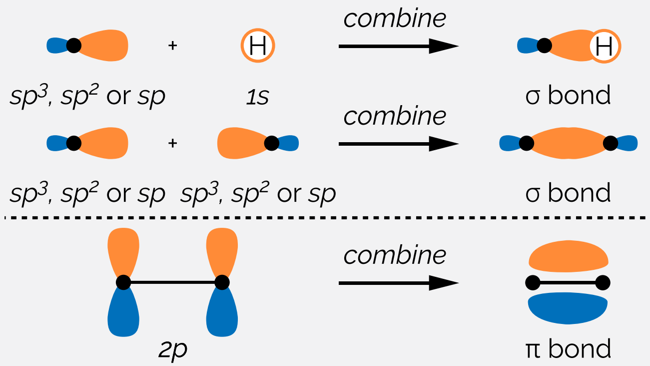


***sp²* hybrid**
Three HAO made from the *2s* & 2 x *2p*. The *sp²* HOAs point to the corners of a triangle. There is a non-hybridised *2p* orbital at 90˚.



***sp* hybrid**
Two HAOs (*2s* + 1 x *2p*). The *sp* HAOs are linear, 180˚ a part. There are two non-hybridised *2p* orbitals 90˚ to each other & sp HAO.

4. Bonds



There two kinds of bond:

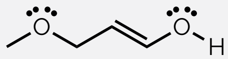
σ bonds - formed from the head-to-head overlap of hybrid atomic orbitals (or HAO and the 1s atomic orbital of hydrogen)

π bonds - formed from the side-to-side overlap of 2p atomic orbitals.

π bonds are weaker than σ bonds as poorer overlap.

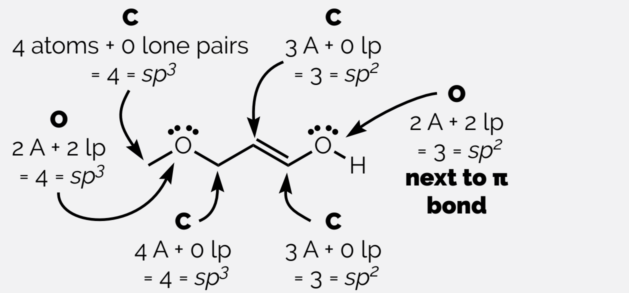
5. Flow chart to determine valence bond model

1. draw Lewis structure



2. assign hybridisation type to each atom

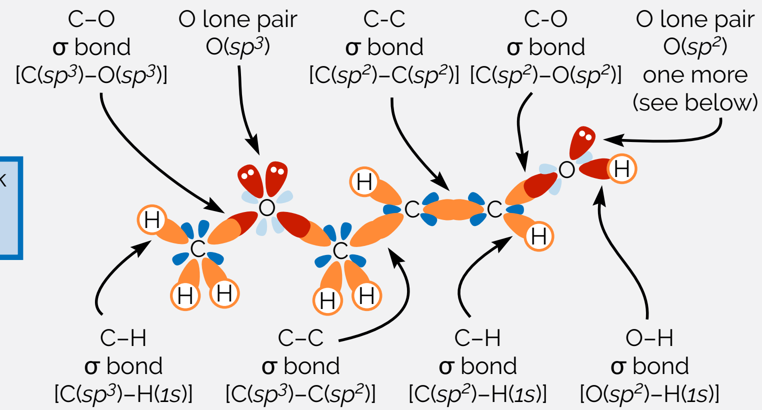
as box 2



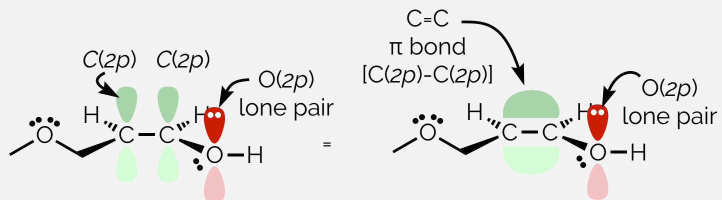
3. describe σ framework by overlap of hybrid orbitals

join atoms with σ bonds

add lone pairs into HAO (unless delocalised)



4. describe any π bonding by overlap of 2p orbitals



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