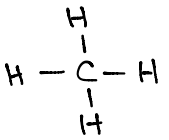
MO theory is <u>really</u> good at predicting the actual electronic properties of molecules

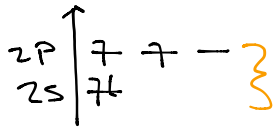
BUT it's really complicated beyond simple diatomic molecules

A different model can be used that lets us easily explain what is observed in molecules and predicted by Lewis structures and VSEPR

As was the case with VSEPR, this approach hinges on identifying electron groups → ALL electron groups on an atom need an <u>EQUAL</u> orbital!



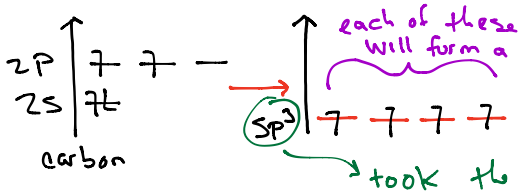
AX_4 → for this molecule to form, we need to have 4 equal atomic orbitals in the valence shell



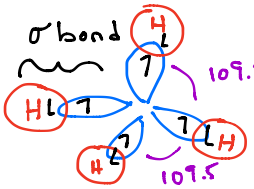
} 4 orbitals but they are not equal!

- also, only 3 orbitals have an electron + we can't break Hund's rule

So what happen is that these 4 orbitals combine to form a Hybrid Atomic Orbital

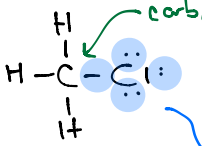


→ took the s orbital and 3 p orbitals and combined them to make a new orbital that has 4 equal lobes



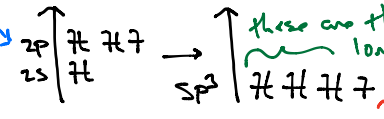
→ the sp^3 hybrid has a tetrahedral shape

CH_3Cl



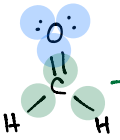
→ carbon is exactly as above

→ chlorine has 4 electron groups (AXE_3 = tetrahedral electron geometry) so need 4 orbitals



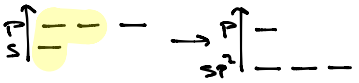
→ this forms a bond with carbon

CH_2O

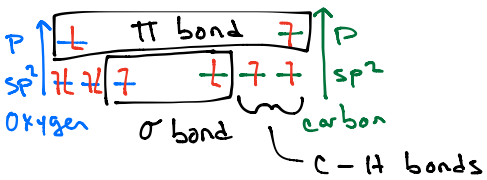


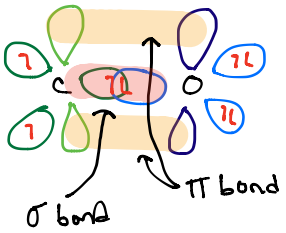
→ AXE_2 → 3 e^- groups so 3 orbitals for the hybrid

→ AX_3 → 3 e^- groups → 3 orbitals for hybrid

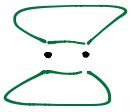


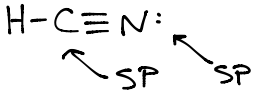
Always take the lowest one first!

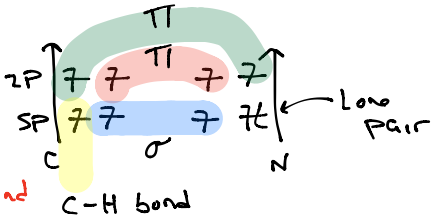




The left over P orbitals are the double bond





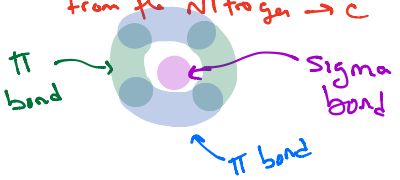


* Every bond starts with a sigma.

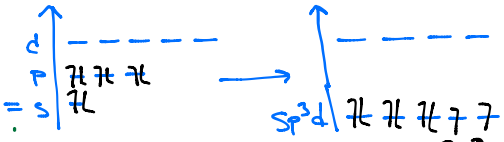
Bond ORDER

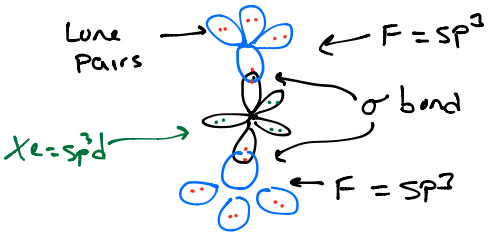
	1	2	3
σ	1	1	1
π	0	1	2

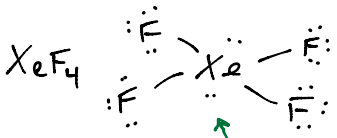
looking at the bond from the Nitrogen → C



5 e^- groups = sp^3d

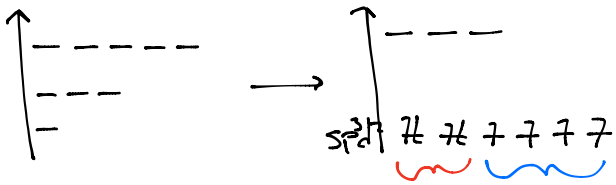






Fluorines are sp^3

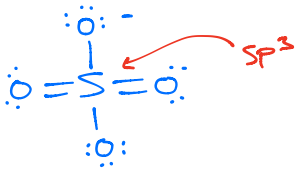
AX$_4$E$_2$ → 6 e$^-$ groups → sp^3d^2



lone pairs

Each orbital makes an Xe-F sigma bond

SO_4^{2-}



sp^3

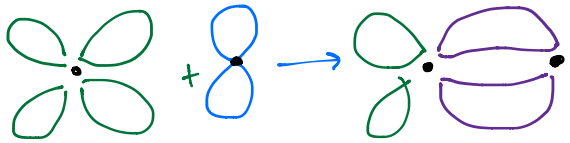
3d

sp^3

These are for the S-O π bonds

These make the S-O σ bonds

D-orbitals can make π bonds

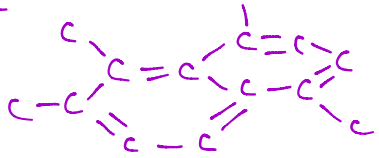


Why does all this matter?

- The shape and bonding character of a molecule dictate its physical properties and reactivity

For example:

Graphene is one form of elemental carbon. It takes on repeating patterns of



Every carbon has a double bond and two resonance structures.

- this means that every C–C bond is partially a double bond

We know that sp^2 carbons (AX_3) have a trig. planar shape

the entire molecule is planar

"conjugated" system of π bonds → this lets graphene transfer electricity!

Punchline: If you're given a molecule, you should be able to:

1. Determine if it is ionic or covalent
2. name it

If covalent:

3. Draw a Lewis structure
4. Determine the shape around each central atom
5. Determine the hybridization of each atom
6. For really simple diatomic molecules, determine the Bond order and number of unpaired electrons (using MO th.)
7. Predict the number of σ & π bonds
8. Associate an energy diagram with your Lewis Structure