

DR. SANDBLOM'S FILL-IN NOTES FOR HYBRIDS...

Now onto a DIFFERENT model:

10.3 Valence Bond Theory &

10.4 Hybridisation of Atomic Orbitals.

This model has some similarities, but remember that they are 2 separate MODELS.

Why do we need this model?

OBSERVATION:

MODEL to predict geometry:

Next, a MODEL to describe how the AOs of C and H are involved in the bonding.

The 2s and 2p atomic orbitals on C cannot give the observed geometry. Also, all of the CH bonds are equivalent, but the AOs are not degenerate.

In this case, the atomic orbitals on a central atom are hybridised or "mixed" to generate hybrid orbitals.

Imagine this as orbitals in a blender.

General Points: the blender does three things:

1.

2.

3.

Examples:

Add an s orbital and a p orbital to the blender:

1.

2.

3.

Add an s orbital and 2 p orbitals to the blender:

1.

2.

3.

Add an s orbital and 3 p orbitals to the blender:

1.

2.

3.

This model ALSO involves overlap of orbitals. Why bother to hybridise before overlapping?

Recall methane: How can the AOs on match the experimental bonding?

Definition: single bond – sigma bond

So, each CH bond

For  $\text{NH}_3$ , predict ARRANGEMENT and hybridisation of N:

Draw energy level diagram and add electrons for N.

Bonding: draw  $\sigma$ -framework

Homework: Draw the  $\sigma$ -framework for water.

For  $\text{BF}_3$ , predict ARRANGEMENT and hybridisation of B:

Draw energy level diagram and add electrons for B.

Bonding: draw  $\sigma$ -framework

Recall: reactivity between  $\text{NH}_3$  and  $\text{BF}_3$  involves the lone pair on N donating electrons to the electron deficient B.

Now: what orbitals are involved?

Draw VSEPR diagram for  $C_2H_4$ .

Hybridisation of central atoms?

Draw energy level diagram and add electrons for C.

Bonding: draw  $\sigma$ -framework

Definition: the double bond

Draw  $\pi$ -system

Homework: Draw the  $\sigma$ -framework and  $\pi$ -system for  $\text{CH}_2\text{O}$  and  $\text{CO}_2$

For  $N_2$ , predict ARRANGEMENT and hybridisation of N:

Draw energy level diagram and add electrons for N

Bonding: draw  $\sigma$ -framework and  $\pi$ -system

Homework: Describe the bonding in  $CH_3CN$  by drawing the  $\sigma$ -framework and the  $\pi$ -system.

Two other types of hybrids are part of this model:

To describe the bonding when we have 5 electron groups in the ARRANGEMENT, add an s orbital, 3 p orbitals, and a d orbital to the blender:

1. 5 hybrids are made:  $sp^3d$
2. Energy will be somewhere between s, 3 p's, and d.
3. Average also looks like a lopsided p orbital. The 5 orbitals will adopt a trigonal bipyramidal ARRANGEMENT. VSEPR TABLE - anytime you have 5 E.G. the central atom will be  $sp^3d$  hybridised.

Similarly, add an s orbital, 3 p orbitals, and 2 d orbitals to the blender:

1. 6 hybrids are made -  $sp^3d^2$
2. Energy will be averaged.
3. Average of also looks like a lopsided p orbital. The 6 orbitals will have an octahedral ARRANGEMENT. VSEPR TABLE - anytime you have 6 E.G. the central atom will be  $sp^3d^2$  hybridised.

Exercises: 26, 34, 36, 38, 40, 42, 44

Homework: Draw the  $\sigma$ -framework and  $\pi$ -system, if applicable, for CO,  $BF_4^-$ ,  $XeF_2$ .

Remember: hybridisation is a model.

Do the atoms really hybridise?

Homework:

1. Identify the shape and hybridisation of the central atom in:  $\text{SeF}_2$ ,  $\text{IF}_3$ ,  $\text{KrF}_2$ ,  $\text{SbF}_6^-$ ,  $\text{KrF}_4$ .
2. Describe the bonding by drawing the  $\sigma$ -framework and  $\pi$ -system for  $\text{BeCl}_2$  and  $\text{O}_2$  (Does this bonding predict a paramagnetic molecule?)

The hybridisation of atomic orbitals is predicted based on the localised electrons as shown in a Lewis diagram. If there is more than one BEST Lewis diagram, resonance allows for the delocalisation of some of the electrons in a Lewis diagram.

## 10.8 Delocalised Molecular Orbitals

The  $\sigma$ -framework of molecules:

However,  $\pi$  bonding is delocalized:

Consider benzene,  $C_6H_6$ :  
Draw best resonance contributors.

*Line Drawings*: shorthand structures

- every corner or bend in the line corresponds to a carbon atom. H's are omitted, but it is assumed that every C has enough H's to have an octet.

Another example: consider the three resonance contributors for carbonate – see Figure 10.30.

Exercise: 63

Additional Exercises: 72, 76 (except e), 80 (except  $CdBr_2$ ), 82, 88