Chem 103, Section F0F
Unit VI - Compounds Part II: Covalent Compounds
Lecture 18

- Valence Bond Theory and Orbital Hybridization
- The Mode of Orbital Overlap and the Types of Covalent Bonds

Lecture 18 - Covalent Bonding

Reading in Silberberg

- Chapter 11, Section 1
  - *VAlence Bond (VB) Theory and Orbital Hybridization*
- Chapter 11, Section 2
  - *The Mode of Orbital Overlap and the Types of Covalent Bonds*

Lecture 18 - Introduction

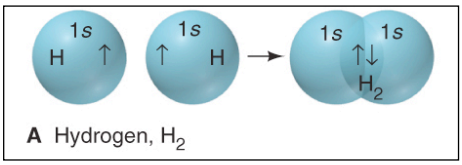
In this lecture we will look into theorys of covent bonding.

- We will look at the Valence Bond (VB) Theory, which resolves the inconsistentcy of what we know about the shapes and orientations of the atomic orbitals (*s, p,* and *d*) with the molecular shapes predicted by the VSEPR Theory.
- We discuss how covalent bonds form when atomic orbitals from different atoms overlap.

Lecture 18 - Valence Bond Theory

Valence bond theory proposes that covalent bonds form when the atomic orbitals of two atoms overlap.

- The combined, overlapping orbitals, contain a total of two electrons.
  - Which, according Pauli's exclusion principle, have opposing spins

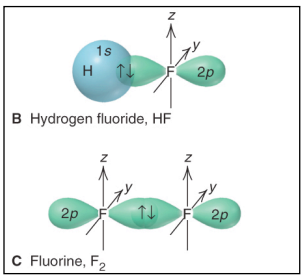


A Hydrogen, H_2

Lecture 18 - Valence Bond Theory

Valence bond theory proposes that covalent bonds form when the atomic orbitals of two atoms overlap.

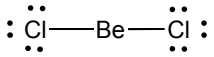
- Every attempt is made to maximize the orbital overlap



Lecture 18 - Valence Bond Theory

Valence bond theory proposes that covalent bonds form when the atomic orbitals of two atoms overlap.

- Hybridization of atomic orbitals provides for molecular shapes that cannot be accommodated by using *s*, *p*, and *d* orbitals.
  - For example, we have seen that the VSEPR theory predicts a linear molecular geometry for $BeCl_2$.



  - It is hard to see how this can be accommodated using *s*, and *p* orbitals.

Lecture 18 - Valence Bond Theory

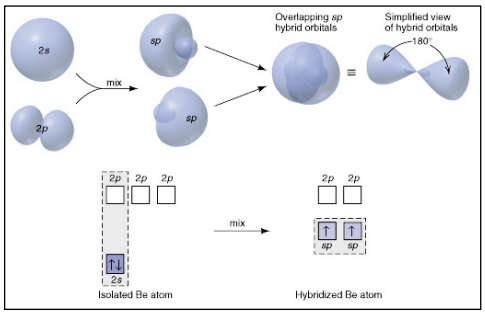
Be: [He]$2s^2$

The *2s* orbital of Be already has two electrons in it.

Cl: [Ne]$3s^2 3p^5$

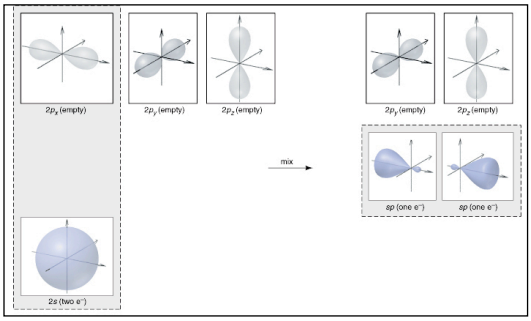
Lecture 18 - Valence Bond Theory

Hybridization of the *2s* with one of the empty *2p* orbitals in Be provides the solution to this problem.



Lecture 18 - Valence Bond Theory

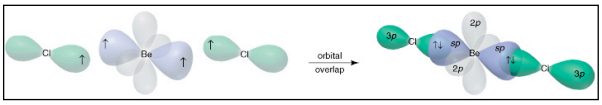
Hybridization of the *2s* with one of the empty *2p* orbitals in Be provides the solution to this problem.



Lecture 18 - Valence Bond Theory

Hybridization of the *2s* with one of the empty *2p* orbitals in Be provides the solution to this problem.

- The half-filled *3p* orbitals from each of the Cl atoms can now each overlap with one of Be's half-filled *2sp* orbitals:



Lecture 18 - Valence Bond Theory

Hybridization:

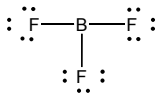
- The *number* of hybrid orbitals obtained *equals* the number of atomic orbitals mixed.
- The *type* of hybrid orbitals obtained *varies* with the types of atomic orbitals mixed.

We have just seen an example of *sp* hybridization with $BeCl_2$, we will now go on to look at some other examples.

Lecture 18 - Valence Bond Theory

sp^2 Hybridization:

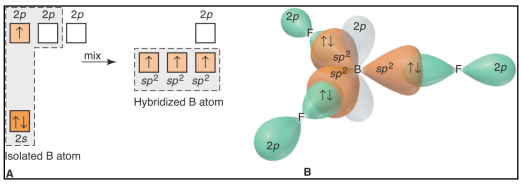
- Example BF_3
  - VSEPR Theory predicts a trigonal planar molecular shape.



Lecture 18 - Valence Bond Theory

sp² Hybridization:

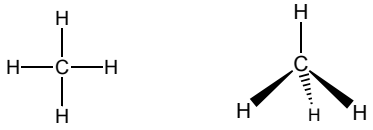
- Example BF_3
  - VSEPR Theory predicts a trigonal planar molecular shape
  - B: [He]$2s^2 2p^1$
  - F: [He]$2s^2 2p^5$



Lecture 18 - Valence Bond Theory

sp³ Hybridization:

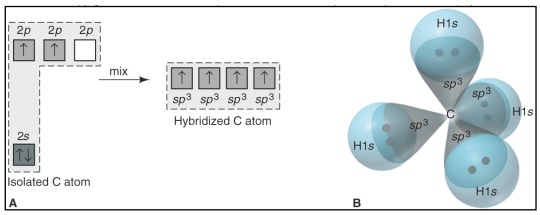
- Example CH_4
  - VSEPR Theory predicts a tetrahedral molecular shape.



Lecture 18 - Valence Bond Theory

sp³ Hybridization:

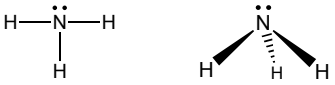
- Example CH_4
  - VSEPR Theory predicts a tetrahedral molecular shape
  - C: [He]$2s^2 2p^2$
  - H: $1s^1$



Lecture 18 - Valence Bond Theory

sp³ Hybridization:

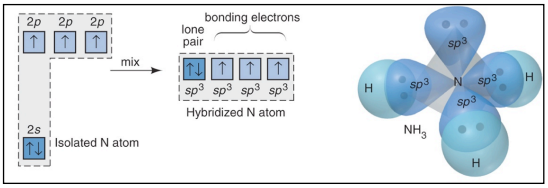
- Example NH_3
  - VSEPR Theory predicts a tetrahedral molecular shape.



Lecture 18 - Valence Bond Theory

sp³ Hybridization:

- Example CH_4
  - VSEPR Theory predicts a tetrahedral molecular shape
  - N: [He]$2s^2 2p^3$
  - H: $1s^1$

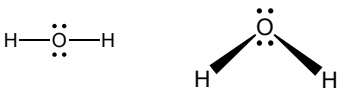


- Hybridized orbitals can also be used to hold non-bonding (lone pair) electrons

Lecture 18 - Valence Bond Theory

sp³ Hybridization:

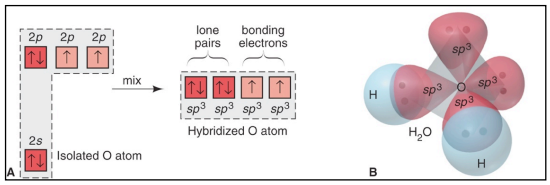
- Example H_2O
  - VSEPR Theory predicts a tetrahedral molecular shape.



Lecture 18 - Valence Bond Theory

*sp*³ Hybridization:

- Example CH_4
  - VSEPR Theory predicts a tetrahedral molecular shape
  - N: [He]$2s^2 2p^3$
  - H: $1s^1$

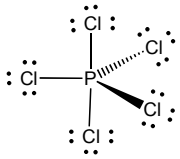


- Hybridized orbitals can also be used to hold non-bonding (lone pair) electrons.

Lecture 18 - Valence Bond Theory

*sp*³*d* Hybridization:

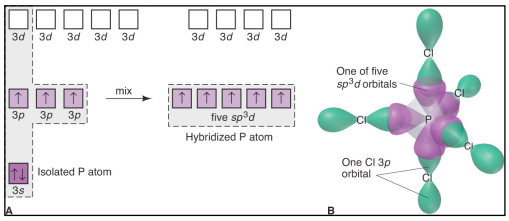
- To go beyond 4 hybridized orbitals the empty *d* orbtals can also be included
- Example PCl_4
  - VSEPR Theory predicts a trigonal bipyramidal molecular shape.



Lecture 18 - Valence Bond Theory

*sp*³*d* Hybridization:

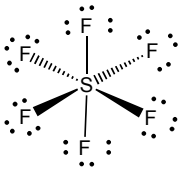
- Example PCl_5
  - VSEPR Theory predicts a trigonal bipyramidal molecular shape
  - P: [Ne] $3s^2 3p^3$
  - Cl: [Ne]$3s^2 3p^5$



Lecture 18 - Valence Bond Theory

*sp*³*d*² Hybridization:

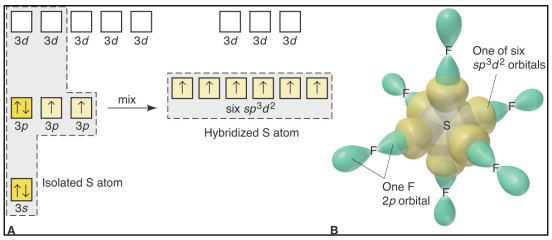
- Example SF_6
  - VSEPR Theory predicts an octahedral molecular shape.



Lecture 18 - Valence Bond Theory

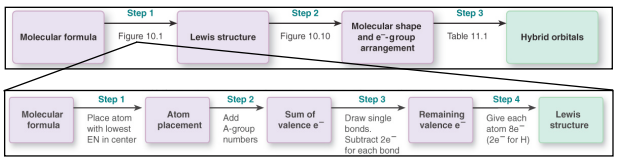
*sp*³*d*² Hybridization:

- Example SF_6
  - VSEPR Theory predicts an octahedral molecular shape
  - S: [Ne] $3s^2 3p^4$
  - F: [He]$2s^2 2p^5$



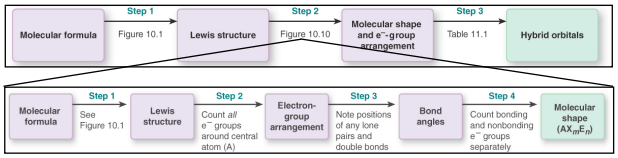
Lecture 18 - Valence Bond Theory

Hybridization and Molecular Shapes



Lecture 18 - Valence Bond Theory

Hybridization and Molecular Shapes



Lecture 18 - Valence Bond Theory

Hybridization and Molecular Shapes

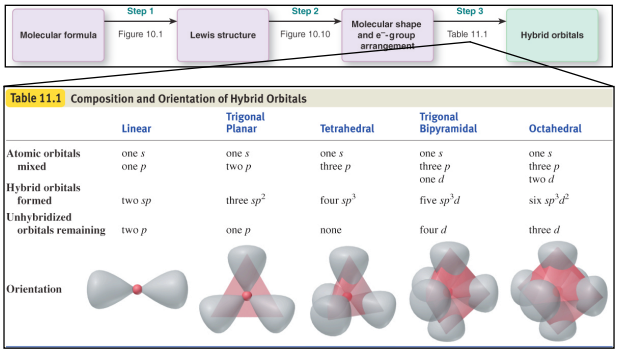


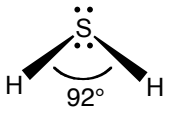
Table 11.1 Composition and Orientation of Hybrid Orbitals

	Linear	Trigonal Planar	Tetrahedral	Trigonal Bipyramidal	Octahedral
Atomic orbitals mixed	one *s* one *p*	one *s* two *p*	one *s* three *p*	one *s* three *p* one *d*	one *s* three *p* two *d*
Hybrid orbitals formed	two *sp*	three sp^2	four sp^3	five sp^3d	six sp^3d^2
Unhybridized orbitals remaining	two *p*	one *p*	none	four *d*	three *d*
Orientation					

Lecture 18 - Valence Bond Theory

Sometimes hybridization does not apply

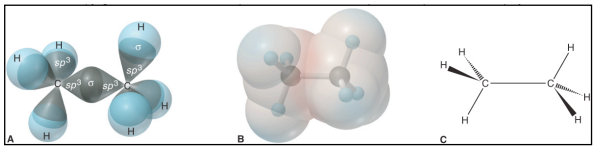
- Example H_2S
  - VSEPR Theory predicts a tetrahedral molecular shape, like H2O.
  - However, the bond angle is closer to that predicted for overlap of the hydrogen *1s* orbtals with non-hybridized *3p* orbitals from the sulfur.



Lecture 18 - Types of Covalent Bonds

σ-Bonds:

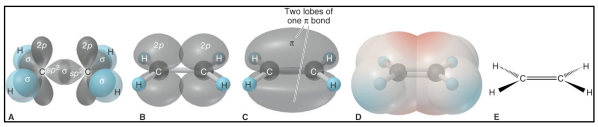
- Arise from end-to-end overlap of *s*, *p*, and *hybridized* sp^x or sp^3d^y orbitals
- All single bonds are σ-bonds.



Lecture 18 - Types of Covalent Bonds

π-Bonds

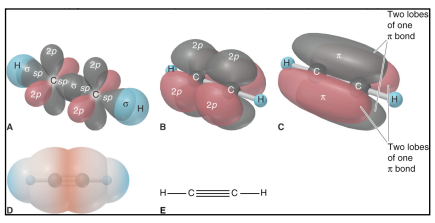
- Multiple bonds involve π-bonds in addition to one σ-bond
- π-Bonds form from side-to-side overlap of *p* or *d* orbitals
- For example:
  - Double-bonds comprise 1 σ-bond and 1 π-bond



Lecture 18 - Types of Covalent Bonds

π-Bonds

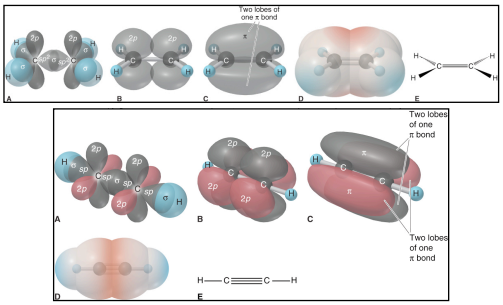
- Mutiple bonds involve π-bonds in addition to one σ-bond
- π-Bonds form from side-to-side overlap of *p* or *d* orbitals
- For example:
  - Triple-bonds comprise 1 σ-bond and 2 π-bonds



Lecture 18 - Types of Covalent Bonds

π-Bonds

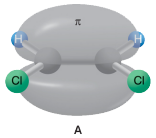
- Have two lobes; the two lobes together make a single π-bond.



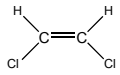
Lecture 18 - Types of Covalent Bonds

π-Bonds restrict rotation about double and triple bonds.

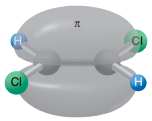
- This can lead to molecules that are *configurational isomer.*
  - The isomers are distinguished as *cis-trans* isomers



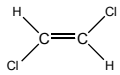
A



cis 1,2-dichloroethene



B



trans 1,2-dichloroethene

Lecture 18 - Question 1

What is the orbital hybridization of t a central atom that has one lone pair and bonds to

A) two other atoms?
B) three other atoms?
C) four other atoms?
D) five other atoms?

Lecture 18 - Question 2

What is the hybridization of the chlorine atom in each of the following polyatomic ions:

A) ClO_2^-
B) ClO_3^-
C) ClO_4^-

Lecture 18 - Question 3

Is this statements true or false:

Two σ-bonds comprise a double bond.

A) True
B) False

Lecture 18 - Question 4

Is this statements true or false:

A triple bond consists of one π-bond and two σ-bonds.

A) True
B) False

Lecture 18 - Question 4

Is this statements true or false:

A πbond consists of two pairs of electrons.

A) True
B) False

Unit VII - Up Next

Lecture 19 - Physical States and Intermolecular Forces

- Overview of physical states and changes
- Description of phase changes
- Types of intermolecular forces

The End