In this lecture we will look into theories of covalent bonding.

- We will look at the Valence Bond (VB) Theory, which resolves the inconsistency 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.

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

- 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 BeCl₂.
  - It is hard to see how this can be accommodated using s, and p orbitals.
Lecture 18 - Valence Bond Theory

Be: [He]2s²

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

Cl: [Ne]3s²3p⁵

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

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 BeCl₂, we will now go on to look at some other examples.

sp² Hybridization:

- Example BF₃
  - VSEPR Theory predicts a trigonal planar molecular shape.
Lecture 18 - Valence Bond Theory

sp² Hybridization:
- Example BF₃
  - VSEPR Theory predicts a trigonal planar molecular shape
  - B: [He]2s²2p¹
  - F: [He]2s²2p⁵

Lecture 18 - Valence Bond Theory

sp³ Hybridization:
- Example CH₄
  - VSEPR Theory predicts a tetrahedral molecular shape.

- C: [He]2s²2p²
- H: 1s¹

Lecture 18 - Valence Bond Theory

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

Lecture 18 - Valence Bond Theory

- Example NH₃
  - VSEPR Theory predicts a tetrahedral molecular shape.

- N: [He]2s²2p³
- H: 1s¹

Lecture 18 - Valence Bond Theory

- Example H₂O
  - VSEPR Theory predicts a tetrahedral molecular shape.

- O: [He]2s²2p⁴
- H: 1s¹
Lecture 18 - Valence Bond Theory

**sp^3 Hybridization:**
- Example CH_4
  - VSEPR Theory predicts a tetrahedral molecular shape
  - N: [He]2s^22p^3
  - H: 1s^1

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

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**sp^3d Hybridization:**
- Example PCl_5
  - VSEPR Theory predicts a trigonal bipyramidal molecular shape
- P: [Ne]3s^23p^3
- Cl: [Ne]3s^23p^5

**sp^3d^2 Hybridization:**
- Example SF_6
  - VSEPR Theory predicts an octahedral molecular shape
- S: [Ne]3s^23p^4
- F: [He]2s^22p^5

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**Hybridization and Molecular Shapes**

**sp^3d Hybridization:**
- To go beyond 4 hybridized orbitals the empty d orbitals can also be included
- Example PCl_5
  - VSEPR Theory predicts a trigonal bipyramidal molecular shape.
Sometimes hybridization does not apply

- Example \( \text{H}_2\text{S} \)
  - VSEPR Theory predicts a tetrahedral molecular shape, like \( \text{H}_2\text{O} \)
  - However, the bond angle is closer to that predicted for overlap of the hydrogen 1s orbitals with non-hybridized 3p orbitals from the sulfur.

\[
\begin{align*}
\text{H} & \quad \text{S} & \quad \text{H} \\
92^\circ \\
\end{align*}
\]
Lecture 18 - Types of Covalent Bonds

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

π-Bonds restrict rotation about double and triple bonds.
• This can lead to molecules that are configurationally isomer.
  - The isomers are distinguished as cis-trans isomers

Lecture 18 - Question 1
What is the orbital hybridization of 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 statement true or false:
Two σ-bonds comprise a double bond.
A) True
B) False

Lecture 18 - Question 4
Is this statement 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 statement true or false:
A bond 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