Guided Practice Activities

**Module:** Bonding

**Section:** Valence Bond Theory - Key
Valence Bond Theory

Activity 1

1. Valence bond theory is a theory that combines empirical data and quantum mechanical ideas to explain the geometric arrangement of bonding and nonbonding electrons around atoms in compounds. The theory is based on the overlap of atomic orbitals. The new mixed orbitals are called hybridized orbitals.

2. Head on overlap of (pure or hybrid) atomic orbitals results in the formation of a sigma bond.

3. Side on overlap of pure atomic orbitals results in the formation of a pi bond.

4. State the types of pure atomic orbitals that are mixed when the following hybrid orbitals are formed: sp, sp², sp³, sp³d, sp³d².

   - sp – one s orbital and one p orbital
   - sp² – one s orbital and two p orbitals
   - sp³ – one s orbital and three p orbitals
   - sp³d – one s orbital, three p orbitals and one d orbital
   - sp³d² – one s orbital, three p orbitals and two d orbitals

Activity 2

1. Complete the following table.

<table>
<thead>
<tr>
<th>Regions of High Electron Density</th>
<th>Electronic Geometry</th>
<th>VB Hybridization</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Linear</td>
<td>sp</td>
</tr>
<tr>
<td>3</td>
<td>Trigonal planar</td>
<td>sp²</td>
</tr>
<tr>
<td>4</td>
<td>Tetrahedral</td>
<td>sp³</td>
</tr>
<tr>
<td>5</td>
<td>Trigonal Bipyramidal</td>
<td>sp³d</td>
</tr>
<tr>
<td>6</td>
<td>Octahedral</td>
<td>sp³d²</td>
</tr>
</tbody>
</table>
Activity 3

1. In Valence Bond Theory hybrid orbitals are degenerate. Use an orbital notation diagram to model this concept starting with the pure atomic orbitals in carbon and ending with the sp^3 hybridized orbitals on the carbon in the compound methane, CH₄.

The carbon in methane has valence electrons in the 2s and 2p orbitals. We know that methane is tetrahedral in shape around the central carbon, therefore we infer that there must be four hybrid orbitals with one electron each ready for the head on overlap with the 1s orbital of the hydrogen atoms. The pure atomic orbitals mix to form four sp^3 orbitals and the four valence electrons are spread across these four hybridized orbitals.

In the diagram below the four pure atomic orbitals (2s and 2p) are shown on the left. After hybridization the four hybrid orbitals are shown on the right. As you can see the four sp^3 orbitals are degenerate (have the same energy) and are higher in energy than the 2s orbital and slightly lower in energy than the 2p orbitals.
Here is visual for understanding how the sp³ orbitals in methane interact with the 1s orbitals in hydrogen:

2. Repeat the exercise in number 1 above for the carbons in ethene (CH₂CH₂).

The carbon in ethene has valence electrons in the 2s and 2p orbitals. We know that ethene is trigonal planar in shape around the central carbon, therefore we infer that there must be three hybrid orbitals with one electron each ready for the head on overlap with the 1s orbital of the hydrogen atoms. Additionally, there must be an electron in a pure p orbital which can perform the side on overlap to form the pi bond between the two carbon atoms in ethene. The pure atomic orbitals mix to form three sp² orbitals and leave one pure 2p orbital. The four valence electrons of carbon are spread across these four different orbitals.

In the diagram below the four pure atomic orbitals (2s and 2p) are shown on the left. After hybridization the three hybrid orbitals and the remaining 2p orbital are shown on the right. As you can see the three sp² orbitals are degenerate (have the same energy) and are higher in energy than the 2s orbital and slightly lower in energy than the 2p orbitals.
3. Repeat the exercise in number 1 above for the carbons in ethyne (CHCH).

The carbon in ethyne has valence electrons in the 2s and 2p orbitals. We know that ethene is linear in shape around the central carbon, therefore we infer that there must be two hybrid orbitals with one electron each ready for the head on overlap with the 1s orbital of the hydrogen atoms. Additionally, there must be electrons in two different, pure p orbitals which can perform the side on overlaps to form the two pi bond between the two carbon atoms in ethyne. The pure atomic orbitals mix to form two sp orbitals and leave two pure 2p orbitals. The four valence electrons of carbon are spread across these four different orbitals.

In the diagram below the four pure atomic orbitals (2s and 2p) are shown on the left. After hybridization the two hybrid orbitals and the remaining 2p orbitals are shown on the right. As you can see the two sp orbitals are degenerate (have the same energy) and are higher in energy than the 2s orbital and lower in energy than the 2p orbitals.
Here is visual for understanding how the orbitals in ethyne interact:

**Forming Ethyne (Acetylene)**

Carbon takes on an sp hybridization with 2 free p orbitals

3 $\sigma$ bonds and 2 $\pi$ bonds form

$\pi$ electrons delocalize into a cylindrical shell density distribution

H–C≡C–H
Activity 4

The purpose of this activity is to deepen your understanding of valence bond theory.

1. Draw the Lewis structure of CO$_2$. Predict the hybridization of the C in the molecule. State the number of sigma and pi bonds in the molecule.

Each carbon is sp hybridized because they each have two areas of electron density around them. There are two sigma bonds (one between each C–O bond) and two pi bonds (one between each C–O bond).

2. What is the hybridization of N in elemental nitrogen, N$_2$? State the number of sigma and pi bonds.

Each nitrogen is sp hybridized because they each have two areas of electron density around them. There are one sigma bond and two pi bonds.

3. Predict the electronic geometry, molecular geometry, bond angles, hybridization, number of σ and π bonds around each atom with an arrow.

The oxygen labeled “A”:

- Electronic Geometry: Tetrahedral
- Molecular Geometry: Bent
- Bond Angles: Less than 109.5° for the angle between H–O–C.
- Hybridization: sp$^3$
- Number of σ bonds: two
- Number of π bonds: zero

The carbon labeled “B”:

- Electronic Geometry: Trigonal Planar
- Molecular Geometry: Trigonal Planar
- Bond Angles: 120°
- Hybridization: sp$^2$
- Number of σ bonds: three
- Number of π bonds: one

The carbon labeled “C”:

- Electronic Geometry: Trigonal Planar
- Molecular Geometry: Trigonal Planar
- Bond Angles: 120°
- Hybridization: sp²
- Number of σ bonds: three
- Number of π bonds: one

The nitrogen labeled "D":

- Electronic Geometry: Tetrahedral
- Molecular Geometry: Trigonal Pyramidal
- Bond Angles: Less than 109.5° for the angles between H–N–C and H–N–H
- Hybridization: sp³
- Number of σ bonds: three
- Number of π bonds: zero