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**CHM 214 ASSIGNMENT.**

1. State the types of hybridization and explain briefly.  Give one example of each.
2. What are the types of overlapping and explain briefly
3. Briefly describe the strength of Sigma and pi bonds
4. Write the Lewis structure of the following compounds
5. CO      ii.         NO2-    iii.        CO2
6. 5. How do we determine the following
7. Bond angle         ii.             Bond Length      iii.            Bond Enthalpy
8. 6. State the postulates of the VSEPR theory

1. **Types of Hybridization**

Based on the types of orbitals involved in mixing, the hybridization can be classified as sp3, sp2, sp, sp3d, sp3d2, sp3d3. Let us now discuss the various types of hybridization along with their examples.
**sp Hybridization**

sp hybridization is observed when one s and one p orbital in the same main shell of an atom mix to form two new equivalent orbitals. The new orbitals formed are called**sp hybridized orbitals.**It forms linear molecules with an angle of 180°

This type of hybridization involves the mixing of one ‘s’ orbital and one ‘p’ orbital of equal energy to give a new hybrid orbital known as an sp hybridized orbital.

sp hybridization is also called diagonal hybridization.

Each sp hybridized orbital has an equal amount of s and p character, i.e., 50% s and p character.

Examples of sp Hybridization: All compounds like beryllium like BeF2.

 **sp2 Hybridization**

**sp2 hybridisation**is observed when one s and two p orbitals of the same shell of an atom mix to form 3 equivalent orbital. The new orbitals formed are called**sp2 hybrid orbitals.**

sp2hybridization is also called trigonal hybridization.

It involves mixing of one ‘s’ orbital and two ‘p’ orbital’s of equal energy to give a new hybrid orbital known as sp2.

A mixture of s and p orbital formed in trigonal symmetry and is maintained at 1200.

All the three hybrid orbitals remain in one plane and make an angle of 120° with one another. Each of the hybrid orbitals formed has 33.33% s character and 66.66% ‘p’ character.

The molecules in which the central atom is linked to 3 atoms and is sp2 hybridized have a triangular planar shape.

E**xamples of sp2 Hybridization**

All the compounds of Boron i.e. BF3,

**sp3 Hybridization**

When one ‘s’ orbital and 3 ‘p’ orbitals belonging to the same shell of an atom mix together to form four new equivalent orbital, the type of hybridization is called a **tetrahedral hybridization or sp3**. The new orbitals formed are called**sp3 hybrid orbitals.**

These are directed towards the four corners of a regular [tetrahedron](https://byjus.com/regular-tetrahedron-formula/) and make an angle of 109°28’ with one another.

 The angle between the sp3 hybrid orbitals is 109.280

Each sp3 hybrid orbital has 25% s character and 75% p character.

Example of sp3 hybridization: [ethane](https://byjus.com/jee/conformations-of-ethane-and-butane/) (C2H6).

**sp3d Hybridization**

sp3d hybridization involves the mixing of 3p orbitals and 1d orbital to form 5 sp3d hybridized orbitals of equal energy. They have trigonal bipyramidal geometry.

The mixture of s, p and d orbital forms trigonal bipyramidal symmetry.

Three hybrid orbitals lie in the horizontal plane inclined at an angle of 120° to each other known as the equatorial orbitals.

The remaining two orbitals lie in the vertical plane at 90 degrees plane of the equatorial orbitals known as axial orbitals.

**Example:**[**Hybridization in Phosphorus pentachloride (PCl5)**](https://byjus.com/chemistry/pcl5-hybridization/)

**sp3d2Hybridization**

sp3d2 hybridization has 1s, 3p and 2d orbitals, that undergo intermixing to form 6 identical sp3d2 hybrid orbitals.

These 6 orbitals are directed towards the corners of an octahedron.

They are inclined at an angle of 90 degrees to one another.

Examples: sulfur hexafluoride, SF6.

**Sp3d3 hybridization :**

*The mixing of one s, three p and  three d- atomic orbitals to form seven equivalent sp3d3 hybrid orbitals of equal energy. This hybridization is known as sp3d3 hybridization.*

**properties :**

1. *Seven sp3d3 hybrid orbitals are directed towards the corners  of a pentagonal bipyramid.*
2. *These are not equivalent hybrid orbitals because five of them are directed towards the corners of a regular pentagon while the remaining two are directed above and below the plane.*
3. *The geometry is pentagonal bipyramidal and bond angle is 720 and 900.*

**Example : formation of IF7**

2. There are two types of overlapping orbitals: sigma (σ) and pi (π). Both bonds are formed from the overlap of two orbitals, one on each atom. σ bonds occur when orbitals overlap between the nuclei of two atoms, also known as the internuclear axis.

σ Bond Formation: Atomic orbitals from two atoms overlap in the region between the nuclei (internuclear axis). Therefore, the resulting electron density of the shared electrons lies in the red region shown in the image.

π bonds occur when two (unhybridized) p-orbitals overlap. The p-orbitals, in one π bond, are located above and below the nuclei of the atoms. By occupying the region of space that is above, below, and on the sides of an atom’s nuclei, two π bonds can form.

π**Bond Formation**: Two unhybridized p-orbitals can overlap so that the electron density of the shared electron pair is described by the π bond depicted on the right.

Both types of overlapping orbitals can be related to bond order. Single bonds have one sigma bond. Double bonds consist of one σ and one π bond, while triple bonds contain one σ and two π bonds.

3. Pi bonds are usually weaker than [sigma bonds](https://en.wikipedia.org/wiki/Sigma_bond). The [C-C](https://en.wikipedia.org/wiki/Carbon%E2%80%93carbon_bond) [double bond](https://en.wikipedia.org/wiki/Double_bond), composed of one sigma and one pi bond, has a bond energy less than twice that of a C-C single bond, indicating that the stability added by the pi bond is less than the stability of a sigma bond. From the perspective of [quantum mechanics](https://en.wikipedia.org/wiki/Quantum_mechanics), this bond's weakness is explained by significantly less overlap between the component p-orbitals due to their parallel orientation. This is contrasted by sigma bonds which form bonding orbitals directly between the nuclei of the bonding atoms, resulting in greater overlap and a strong sigma bond.

4. Lewis Structure of CO.



Lewis Structure of CO2



Lewis Structure of NO2-.

3.

5.

There are three basic steps to determining the bond angles in a molecule:

**Explanation:**

**1. Write the Lewis dot structure for the molecule.**

Assume that you must determine the bond angles in BF3.

B is less electronegative than F, so B becomes the central atom.

If we have three F atoms, that means that we are going to use all three electrons from the B.

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This gives us three bonding pairs of electrons and 0 nonbonding pairs.

Thus, the **steric number, SN** — the number of non-bonding and bonding electron groups (**Note:** single, double, and triple bonds all count as one electron group).

The SN is also known as the number of **ELECTRON DOMAINS**.

**2. Use the steric number and VSEPR theory to determine the electron domain geometry of the molecule.**

To get the VSEPR geometry, imagine that there is a sphere around the central atom.

Place the electron pairs on the surface of the sphere so that they are as far apart as possible.

This is how two to six electron domains arrange themselves on the surface of a sphere.

Electron Domain Geometries

Three electron groups arrange themselves evenly around the equator of the sphere to give a trigonal planar shape.

3. Use the [VSEPR](http://socratic.org/chemistry/covalent-bonds-and-formulas/the-geometrical-arrangement-of-electrons-and-molecular-shape-vsepr) shape to determine the angles between the electron domains.

From elementary math, we know that a circle is composed of 360 °.

We divide this number by the number of electron domains and get

360°3=120°.

Thus, the bond angles in BF3 are 120 °.

2.Determination of Bond Length: The **length** of the **bond** is **determined** by the number of bonded electrons (the **bond** order). The higher the **bond** order, the stronger the pull between the two atoms and the shorter the **bond length**. Generally, the **length** of the **bond** between two atoms is approximately the sum of the covalent radii of the two atoms.

**3.Determination of Bond Energy( Enthalpy).**

**1.Define the equation for calculating bond energy.** Bond energy is defined by the sum of all of the bonds broken minus the sum of all of the bonds formed: ΔH = ∑H(bonds broken) - ∑H(bonds formed). ΔH is the change in bond energy, also referred to as the bond enthalpy and ∑H is the sum of the bond energies for each side of the equation.[[3]](https://www.wikihow.com/Calculate-Bond-Energy#_note-3)

This equation is a form of Hess’s Law.

The unit for bond energy is kilojoules per mol or kJ/mol.[[4]](https://www.wikihow.com/Calculate-Bond-Energy#_note-4)

**2.Draw the chemical equation showing all of the bonds between molecules.** When given a reaction equation simply written with chemical symbols and numbers, it is helpful to draw this equation out, illustrating all of the bonds formed between the various elements and molecules. This visual representation will allow you to easily count all of the bonds that break and form on the reactant and product sides of the equation.

Remember, the left side of the equation is all of the reactants and the right side is all of the products.

Single, double, and triple bonds have different bond energies, so be sure to draw your diagram with the correct bonds between elements.

For example, if you were to draw out the following equation for a reaction between 2 hydrogen and 2 bromine: H2(g) + Br2(g) ---> 2 HBr(g), you would get: H-H + Br-Br ---> 2 H-Br. The hyphens represent single bonds between the elements in the reactants and the products.

**3.Know the rules for counting broken and formed bonds.** In most cases, the bond energies you will be using for these calculations will be averages. The same bond can have a slightly different bond energy based on the molecule it is formed in; therefore, average bond energies are generally used..

A single, double, and triple bond are all treated as 1 break. They all have different bond energies, but count as only a single break.

The same is true for the formation of a single, double, or triple bond. It will be counted as single formation.

For our example, all of the bonds are single bonds.

**4.Identify the bonds broken on the left side of the equation.** The left side contains the reactants. These will represent all of the broken bonds in the equation. This is an endothermic process that requires the absorption of energy to break the bonds.

For our example, the left side has 1 H-H bond and 1 Br-Br bond.

**5.Count the bonds formed on the right side of the equation.** The right side contains all of the products. These are all of the bonds that will be formed. This is an exothermic process that releases energy, usually in the form of heat.[[9]](https://www.wikihow.com/Calculate-Bond-Energy#_note-9)

For our example, the right side has 2 H-Br bonds.

**\Calculating the Bond Energy Part 2**

1. **Look up the bond energies of the bonds in question.** There are many tables that have information on the average bond energies for a specific bond. These tables can be found online or in a chemistry book. It is important to note that these bond energies are always for molecules in a gaseous state.

For our example, you need to find the bond energy for an H-H bond, a Br-Br bond, and an H-Br bond.

H-H = 436 kJ/mol; Br-Br = 193 kJ/mol; H-Br = 366 kJ/mol.

To calculate bond energy for molecules in a liquid state, you need to also look up the enthalpy change of vaporization for the liquid molecule. This is the amount of energy needed to convert the liquid into a gas.[[12]](https://www.wikihow.com/Calculate-Bond-Energy#_note-12) This number is added to the total bond energy.

For example: If you were given liquid water, you would need to add the enthalpy change of vaporization of water (+41 kJ) to the equation.

**2**

**Multiply the bond energies by the number of bonds broken.** In some equations, you may have the same bond broken multiple time. For example, if 4 atoms of hydrogen are in the molecule, then the bond energy of hydrogen must be counted 4 times, or multiplied by 4.

In our example, there is only 1 bond of each molecule, so the bond energies are simply multiplied by 1.

H-H = 436 x 1 = 436 kJ/mol

Br-Br = 193 x 1 = 193 kJ/mol

**3**

**Add up all of the bond energies of the broken bonds.** Once you have multiplied the bond energies by the number of the individual bonds, you need to then sum all of the bonds on the reactant side.[[15]](https://www.wikihow.com/Calculate-Bond-Energy#_note-15)

For our example, the sum of the bonds broken is H-H + Br-Br = 436 + 193 = 629 kJ/mol.

**4**

**Multiply the bond energies by the number of bonds formed.** Just as you did for the bonds broken on the reactant side, you will multiply the number of bonds formed by its respective bond energy.[[16]](https://www.wikihow.com/Calculate-Bond-Energy#_note-16) If you have 4 hydrogen bonds formed, you would need to multiply that bond energy by 4.

For our example we have 2 H-Br bonds formed, so the bond energy of H-Br (366 kJ/mol) will be multiplied by 2: 366 x 2 = 732 kJ/mol.

**5**

**Add up all of the formed bond energies.** Again, like you did with the bonds broken, you will add up all of the bonds formed on the product side.[[17]](https://www.wikihow.com/Calculate-Bond-Energy#_note-17) Sometimes you will only have 1 product formed and can skip this step.

In our example, there is only 1 product formed, so the energy of the bonds formed is simply the energy of the 2 H-Br bonds or 732 kJ/mol.

**6**

**Subtract the formed bonds from the broken bonds.** Once you have summed all of the bond energies for both sides, simply subtract the formed bonds from the broken bonds. Remember the equation: ΔH = ∑H(bonds broken) - ∑H(bonds formed). Plug in the calculated values and subtract.

For our example: ΔH = ∑H(bonds broken) - ∑H(bonds formed) = 629 kJ/mol - 732 kJ/mol = -103 kJ/mol.

**7**

**Determine whether the entire reaction was endothermic or exothermic.** The final step to calculating bond energy is to determine whether the reaction releases energy or consumes energy. An endothermic (one that consumes energy) will have a final bond energy that is positive, while an exothermic reaction (one that releases energy) will have a negative bond energy.

In our example, the final bond energy is negative, therefore, the reaction is exothermic.

**Postulates of VSEPR Theory**:

The postulates of the VSEPR theory are listed below

In polyatomic molecules (i.e. molecules made up of three or more atoms), one of the constituent atoms is identified as the central atom to which all other [atoms belonging to the molecule](https://byjus.com/chemistry/atoms-and-molecules/) are linked.

The total number of valence shell electron pairs decides the shape of the molecule.

The electron pairs have a tendency to orient themselves in a way that minimizes the electron-electron repulsion between them and maximizes the distance between them.

The valence shell can be thought of as a sphere wherein the electron pairs are localized on the surface in such a way that the distance between them is maximized.

Should the central atom of the molecule be surrounded by bond pairs of electrons, then, the asymmetrically shaped molecule can be expected.

Should the central atom be surrounded by both lone pairs and bond pairs of electrons, the molecule would tend to have a distorted shape.

 The VSEPR theory can be applied to each [resonance structure](https://byjus.com/chemistry/resonance-structures/) of a molecule.

 The strength of the repulsion is strongest in two lone pairs and weakest in two bond pairs.

If electron pairs around the central atom are closer to each other, they will repel each other. This results in an increase in the energy of the molecules.

If the electron pairs lie far from each other, the repulsions between them will be less and eventually, the [energy of the molecule](https://byjus.com/physics/energy-level/) will be low.