**14.2 Hybridization**

**Learning objectives**

* Understand what is meant by hybridisation
* Predict the hybridisation of atoms in a molecule

**Understandings:**

* A hybrid orbital results from the mixing of different types of atomic orbitals on the same atom.

**Inquiry: Carbon has a ground state electron configuration 1s22s22px12py1. How does it form four similar covalent bonds in methane?**

In all its covalently bonded compounds, carbon forms four covalent bonds. Yet the electron configuration in the carbon atom, would not predict this as it has only two singly occupied orbitals available for bonding.

C atomic number = 6 electron configuration: 1s22s22px12py1, **the ground state** electron configuration. The ground-state electron configuration changes during bonding. A process known as **excitation** occurs in which an electron is promoted within the atom from the 2s orbital to the vacant 2p orbital. The atom now has four singly occupied orbitals available for bonding and the amount of energy put in to achieve this is more than compensated by the extra energy released on forming four bonds.



Ground state electron configuration C excited state electron conﬁguration

**Hybridization**

Hybridization involves mixing atomic orbitals to form new hybrid atomic orbitals. The process of excitation explains how carbon is able to form four covalent bonds but the orbitals are not all the same: there is **one s** orbital, and **three p** orbitals at a **slightly higher energy.** So if these were used in forming the covalent bonds, we would expect unequal bonds. The fact that methane, CH4, has four identical carbon–hydrogen bonds suggests that these orbitals have been changed and somehow made equal during the bonding process.

In essence unequal atomic orbitals within an atom mix to form **new hybrid atomic orbitals** which are the same as each other, but different from the original orbitals. This mixing of orbitals is known as **hybridization.**

Hybridisation is the mixing of atomic orbitals in a particular atom to produce a new set of orbitals (the same number as originally) that have characteristics of the original orbitals and are better arranged in space for covalent bonding.

Hybrid orbitals have different energies, shapes, and orientation in space from their parent orbitals and are able to form stronger bonds by allowing for greater overlap.

* Hybridization of **one s** orbital with **three p** orbitals produces *four* so-called **sp3 hybrid orbitals** that are equal to each other. Their shape and energy have properties of both s and p, but are more like p than s.
* Hybridization of **one s** orbital with **two p orbitals** will produce three equal **sp2 hybrid orbitals**.
* Finally, hybridization of **one s** orbital with **one p** orbital will produce two equal **sp hybrid orbitals.**

When carbon forms four single bonds, it undergoes sp3 hybridization, producing four equal orbitals.



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What is the shape of p-atomic orbitals? Dumbbell shape can overlap sideways, head-on (

What are the angles between the p atomic orbitals? Mutual right angles

What is the shape of s orbitals? spherical

The four sp3 hybrid orbitals have the same energy and they are degenerate. They orientate themselves at 109.5°, forming a tetrahedron. Each hybrid orbital overlaps with the atomic orbital of another atom forming four sigma bonds.

**Sp2 hybridization**

When carbon forms a double bond, it undergoes sp2 hybridization, producing three equal orbitals.



These orbitals orientate themselves at 120°, forming a triangular planar shape. Each hybrid orbital overlaps with a neighbouring atomic orbital, forming three sigma bonds.

For example, ethene, C2H4.



*Structure of ethene. The three sp2 hybrid orbitals on each carbon atom form a triangular planar shape, overlapping to form one C–C and two C–H sigma bonds. The unhybridized p orbitals on each carbon atom overlap to form a pi bond.*

**sp hybridization**

When carbon forms a triple bond, it undergoes sp hybridization, producing two equal orbitals.



These orbitals orientate themselves at 180°, giving a linear shape. Overlap of the two hybrid orbitals with other atomic orbitals forms two sigma bonds.

Each carbon has two unhybridized p orbitals that are orientated at 90° to each other. As these overlap each other sideways, two pi bonds form. These coalesce into a cylinder of negative charge around the atom, making the molecule susceptible to attack by electrophilic reagents.

For example, ethyne, C2H2.



**Lone pairs can be involved in hybridization too**

Non-bonding pairs of electrons can also take part in hybridization. For example, in ammonia, NH3, the non-bonding pair on the N atom resides in a sp3 hybrid orbital.

**Hybridization can also be used to predict molecular shape**

The relationship is as follows:

* tetrahedral arrangement ↔ sp3 hybridized
* triangular planar arrangement ↔ sp2 hybridized
* linear arrangement ↔ sp hybridized.

 So now we can look again at the geometric arrangement of the electron domains predicted by VSEPR theory, and deduce the hybridization involved.



 Rule of the thumb

Subtract 2-3 degrees for every lone pair from the electron domain geometry



**Questions**

1. Urea is present in solution in animal urine. What is the hybridization of C and N in the molecule, and what are the approximate bond angles?

C sp2 120

N sp3 107

1. a. Explain the term ‘hybridisation’. [2]

b. Predict the hybridisation of the carbon atoms in ethene (C2H4) and ethyne (C2H2). [2]

(C2H4) sp2shape trigonal planar , 120 (C2H2) sp ; linear, 180

c. Explain, by reference to ethene and ethyne, what is meant by the terms ‘sigma bond’ and ‘pi bond’. [4]

 sigma – 2C-H and 1 pi C=C

1. a .Use the valence shell electron pair repulsion theory to predict the shapes and bond angles of the following molecules or ions:

 i SO42−

ii XeF4

iii SF4 [6]

b. Explain whether XeF4 is polar or non-polar. [2]

 c. Explain how you would expect the S–O bond length in SO42− to compare with that in SO2. [2]

1. But-2-ene is a straight-chain alkene with formula C4H8. The molecule contains both sigma and pi bonds.
2. Explain the formation of the pi bond. (2) 

(b) For each of the carbon atoms, C1 and C2, identify the type of hybridization shown.