# 14.2 Hybridization

## Understandings:

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

## Applications and skills:

- Explanation of the formation of $sp^3$, $sp^2$, and sp hybrid orbitals in methane, ethene, and ethyne.
- Identification and explanation of the relationships between Lewis (electron dot) structures, electron domains, molecular geometries, and types of hybridization.

***Guidance***

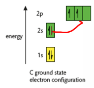
*Students need only consider species with $sp^3$, $sp^2$, and sp hybridization.*

What Group is carbon in? 14

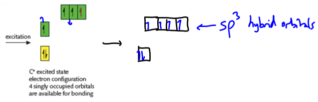
How many valence electrons does it have? 4

How many does it want to gain through covalent bonding? 4

How many half-filled orbitals does it have to make these covalent bonds?



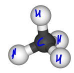

The fact that it forms 4 bonds means that 1 electron from the 2s orbital must be promoted to the empty p orbital :



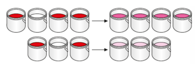

This process is called excitation . The energy require to do it is compensated by the energy released when the covalent bonds are formed.

The problem faced now is that we would expect unequal bonds as one of them is formed using an s-orbital. The fact that methane has 4 equal bond lengths indicates that this is not the case.

We find that a process of hybridisation occurs to form 4 hybrid orbitals of a new energy, shape and orientation are formed.

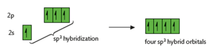


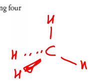

The exact nature of these orbitals depend on the type of orbitals that have been hybridised to form them as with mixing paints:



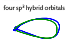
### $sp^3$ hybridization

When carbon forms four single bonds, it undergoes $sp^3$ hybridization, producing four equal orbitals.

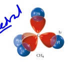



What is the shape of one hybrid orbital ? -->

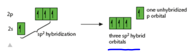


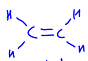
What geometry will be formed by 4 identical hybrid orbitals ? --> Tetrahedral



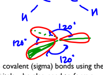

### $sp^2$ hybridization

If a carbon is only bonded to 3 other atoms then it forms three $sp^2$ hybrid orbitals :

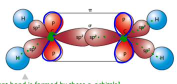


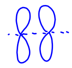




What geometry will be formed by 3 identical hybrid orbitals ? -->




If we draw the example of ethene ($C_2H_4$) we see that after forming 3 covalent (sigma) bonds using the 3 hybrid orbitals, we coincidentally have 2 parallel unhybridised p-orbitals who also need to form a covalent bond:



What kind of covalent bond is formed by these p-orbitals?

So we find that a double bond is always formed from... 1 sigma and 1 pi bond.

### sp hybridization

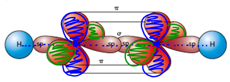
When carbon forms a triple bond, it undergoes sp hybridization, producing two equal orbitals.


ethyne

H—C≡C—H

What geometry will be formed by 2 identical hybrid orbitals ? -->

If we draw the example of ethyne ($C_2H_2$) we see that after forming 2 covalent (sigma) bonds using the 2 hybrid orbitals, we coincidentally have 4 parallel unhybridised p-orbitals who also need to form a covalent bond:

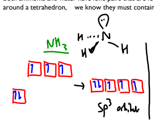


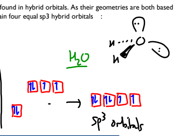

What kind of covalent bond is formed by these p-orbitals? π bond

So we find that a triple bond is always formed from... 1 sigma bond + 2 π bonds

## Lone pairs can also be involved in hybridisation

Both ammonia and water have lone pairs that are found in hybrid orbitals. As their geometries are both based around a tetrahedron, we know they must contain four equal sp3 hybrid orbitals :

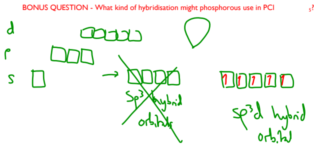



| Number of electron domains | Electron domain geometry | Molecular geometry | Example | Hybridization |
|---|---|---|---|---|
| 2 | linear | linear | $CO_2$ O=C=O | |
| 3 | planar triangular | planar triangular | $BCl_3$ | |
| 3 | planar triangular | V-shaped | $SO_2$ | |
| 4 | tetrahedral | tetrahedral | $CH_4$ | |
| 4 | tetrahedral | pyramidal | $NH_3$ | |
| 4 | tetrahedral | V-shaped | $H_2O$ | |

* We can use this knowledge to relate hybridisation and geometry information.

BONUS QUESTION - What kind of hybridisation might phosphorous use in $PCl_5$?

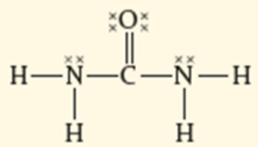


## Worked example

Urea $H_2N-C(=O)-NH_2$ 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?

### Solution

Start with the Lewis (electron dot) structure.



Because there are three electron domains around the C atom, they are arranged in a triangular planar shape with angles of 120°. The C atom must be $sp^2$ hybridized to give this shape. There are four electron domains around each N atom, so they are arranged tetrahedrally. The N atoms must be $sp^3$ hybridized to give this shape.

## Exercises

**43** What is the difference in spatial distribution between electrons in a pi bond and electrons in a sigma bond?

**44** Give examples of sigma bonds in molecules that form from overlap of the following orbitals. The first one is completed for you as an example.

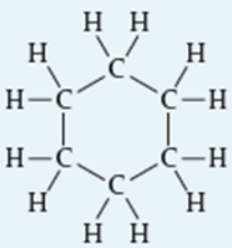
**(a)** s–s: <u>answer</u> H–H in $H_2$

**(b)** s–p **(c)** p–p end-on **(d)** $sp^3$–s **(e)** $sp^2$–s
**(f)** sp–s **(g)** $sp^2$–p

**45** What hybridization would you expect for the coloured atom in each of the following?

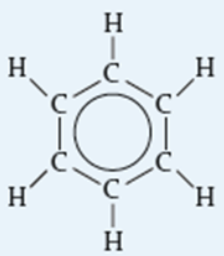
**(a)** $H_2C{=}O$ **(b)** $BH_4^-$ **(c)** $SO_3$
**(d)** $BeCl_2$ **(e)** $CH_3COOH$

**46** Cyclohexane $C_6H_{12}$



has a puckered, non-planar shape whereas benzene

$C_6H_6$



is planar.

Explain this difference by making reference to the C–C–C bond angles and the type of hybridization of carbon in each molecule.

Practice questions

1 Which bonds are arranged in order of increasing polarity?

A H–F < H–Cl < H–Br < H–I
B H–I < H–Br < H–F < H–Cl
C H–I < H–Br < H–Cl < H–F
D H–Br < H–I < H–Cl < H–F

2 Which row correctly describes the bonding type and melting point of carbon and carbon dioxide?

| | Carbon | | Carbon dioxide | |
|---|---|---|---|---|
| A | covalent bonding | high melting point | covalent bonding | low melting point |
| B | ionic bonding | low melting point | ionic bonding | high melting point |
| C | ionic bonding | high melting point | ionic bonding | low melting point |
| D | covalent bonding | low melting point | covalent bonding | high melting point |

6 Which compound forms hydrogen bonds in the liquid state?

A $C_2H_5OH$ B $CHCl_3$ C $CH_3CHO$ D $(CH_3CH_2)_3N$

7 Which molecule has a non-bonding (lone) pair of electrons around the central atom?

A $BF_3$ B $SO_2$ C $PCl_5$ D $SiF_4$

8 Which species does not have delocalized electrons?

A $NO_3^-$ B $NO_2^-$ C $O_3$ D $C_3H_6$

9 Which species contain a dative covalent bond?

I HCHO
II CO
III $H_3O^+$

A I and II only B I and III only C II and III only D I, II, and III

10 Which molecule has an octahedral shape?

A $SF_6$ B $PCl_5$ C $XeF_4$ D $BF_3$

11 Which statements about $\sigma$ and $\pi$ bonds are correct?

I $\sigma$ bonds result from the axial overlap of orbitals.
II $\sigma$ bonds only form from s orbitals.
III $\pi$ bonds result from the sideways overlap of parallel p orbitals.

A I and II only B I and III only C II and III only D I, II, and III

12 In which substance does a carbon atom have $sp^2$ hybridization?

A 2-methylbutan-1-ol B propyne, $CH_3CCH$ C $C_{60}$, fullerene D diamond

13 The Lewis structure of $XeF_2$ contains two bonding pairs of electrons and three non-bonding pairs of electrons (lone pairs) around the central xenon atom. What is the shape of the $XeF_2$ molecule?

A bent B trigonal bipyramidal
C square planar D linear

18 Carbon and silicon belong to the same group of the periodic table.

(a) Describe and compare three features of the structure and bonding in the three allotropes of carbon: diamond, graphite, and $C_{60}$ fullerene. (6)

(b) Both silicon and carbon form oxides.

(i) Describe the structure and bonding in $SiO_2$. (2)

(ii) Explain why silicon dioxide is a solid and carbon dioxide is a gas at room temperature. (2)

(c) Describe the bonding within the carbon monoxide molecule. (2)

(d) Describe the delocalization of pi ($\pi$) electrons and explain how this can account for the structure and stability of the carbonate ion, $CO_3^{2-}$. (3)

(e) Explain the meaning of the term *hybridization*. State the type of hybridization shown by the carbon atoms in carbon dioxide, diamond, graphite, and the carbonate ion. (5)

*(Total 20 marks)*

21 $SF_2$, $SF_4$ and $SF_6$ have different shapes. Draw their Lewis (electron dot) structures and use the VSEPR theory to predict the name of the shape of each molecule. (6)

22 (a) Draw the Lewis (electron dot) structures, state the shape, and predict the bond angles for the following species.

(i) $PCl_3$ (3)

(ii) $NH_2^-$ (3)

(iii) $XeF_4$ (3)

(b) (i) Compare the formation of a sigma ($\sigma$) and a pi ($\pi$) bond between two carbon atoms in a molecule. (2)

(ii) Identify how many sigma and pi bonds are present in propene, $C_3H_6$. (2)

(iii) Deduce all the bond angles present in propene. (2)

(iv) Explain how the concept of hybridization can be used to explain the bonding in the triple bond present in propyne. (3)

*(Total 18 marks)*

23 (a) Draw the Lewis (electron dot) structures, state the shapes, and predict the bond angles for the following species.

(i) $SiF_6^{2-}$ (3)

(ii) $NO_2^+$ (3)

(b) Explain, using diagrams, why $NO_2$ is a polar molecule but $CO_2$ is a non-polar molecule. (3)

(c) Describe the structure and bonding in silicon dioxide. (2)

(d) Consider the molecule $HCONH_2$.

(i) State the name of the compound and draw its structural formula, showing all the bonds present. (2)

(ii) Explain the term *hybridization*. (1)

(iii) Describe how sigma and pi bonds form. (2)

(iv) State the type of hybridization of the carbon and nitrogen atoms in $HCONH_2$. (2)

*(Total 18 marks)*

Homework → Topic 0 Repaso de química

Q 9, 10, 18, 18

Bonds

→ 2 types

→ $\sigma$ bond is stronger

→ Covalent → Sigma ($\sigma$) → overlap on bond axis

→ Pi ($\pi$) → sideways → 2 p orbitals

→ Double bond = 1 $\sigma$ + 1 $\pi$

Hybridisation

→ Hybrid orbitals

→ sp, $sp^2$, $sp^3$

→ excitation of s electron

→ $CH_4$ methane → tetrahedral