

Short cut to decide Hybridization state

(1) Hybridization in an atom of second period = sp^{n-1}

Where, n = No. of bonds made by the atom + no. of lone pairs on the atom
= No. of atoms bonded to the atom + no. of lone pairs on the atom

Fact- Lone pair of electrons usually occupy hybridized orbitals.

For example, in following compound-



Hybridization in nitrogen atom = sp^{n-1}

Here, n = no. of bonds made by the atom + no. of lone pairs on the atom
= 1 (triple bond) + 1 (Lone pair)
= 2

\therefore Hybridization in nitrogen atom = sp^{2-1}
= sp

Hybridization in carbon atom of CN group = sp^{n-1}

Here, n = no. of bonds made by the atom + no. of lone pairs on the atom
= 1 (triple bond) + 1 (single bond) + 0 (Lone pair)
= 2

\therefore Hybridization in carbon atom of CN group = sp^{2-1}
= sp

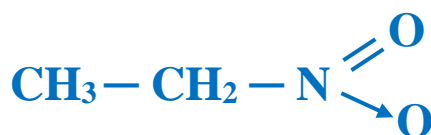
Similarly, for following molecule,



Hybridization in oxygen atom = sp^{n-1}

Here, n = no. of bonds made by the atom + no. of lone pairs on the atom
= 2 (single bond) + 2 (Lone pair)
= 4

\therefore Hybridization in oxygen atom = sp^{4-1}
= sp^3



Here, Hybridization in nitrogen atom = sp^{n-1}

Here, n = no. of bonds made by the atom + no. of lone pairs on the atom
= 2 (single bond) + 1 (double bond)
= 3

$$\begin{aligned} \therefore \text{Hybridization in nitrogen atom} &= sp^{3-1} \\ &= sp^2 \end{aligned}$$

Hybridization in doubly bonded oxygen atom = sp^{n-1}

$$\begin{aligned} \text{Here, } n &= \text{no. of bonds made by the atom} + \text{no. of lone pairs on the atom} \\ &= 1 \text{ (double bond)} + 2 \text{ (lone pairs)} \\ &= 3 \end{aligned}$$

$$\begin{aligned} \therefore \text{Hybridization in doubly bonded oxygen atom} &= sp^{3-1} \\ &= sp^2 \end{aligned}$$

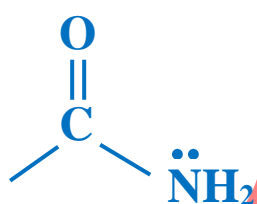
Hybridization in coordinate bonded oxygen atom = sp^{n-1}

$$\begin{aligned} \text{Here, } n &= \text{no. of bonds made by the atom} + \text{no. of lone pairs on the atom} \\ &= 1 \text{ (single bond)} + 2 \text{ (lone pairs)} \\ &= 3 \end{aligned}$$

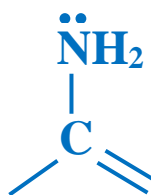
$$\begin{aligned} \therefore \text{Hybridization in oxygen atom coordinate bonded} &= sp^{3-1} \\ &= sp^2 \end{aligned}$$

Exceptions-

(1) If a lone pair of electrons is in conjugation with pi bond, then it tends to occupy unhybridized p-orbital rather than hybridized orbitals. For example, in acid amides and enamines, the actual hybridization state of nitrogen is sp^2 , but not expected hybridization state of sp^3 .

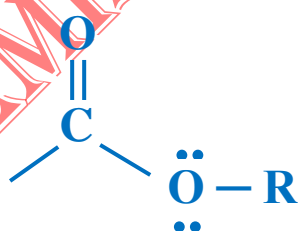


Acid amide

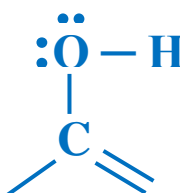


Enamine

Similarly, in esters and enols, the actual hybridization state of oxygen is sp^2 , but not expected hybridization state of sp^3 .



Ester



Enol

It is because of the fact that, unhybridized p-orbital overlaps better with pi electron system resulting in more lowering in energy and therefore, more stabilization than the hybridized orbitals.

Similarly, when the lone pair electrons is incorporated with pi-electrons of aromatic system, then it tends to occupy unhybridized p-orbital, rather than hybridized orbitals. For example, in following cases, the actual hybridization state of nitrogen and oxygen is sp^2 , but not expected hybridization state of sp^3 .

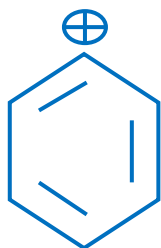


Pyrrole



Furan

(3) In phenyl carbocation, positively charged carbon is bonded with two atoms and has no lone pair. Hence, using short cut method it should be sp hybridized, but due to geometric constrain it is sp^2 hybridized.



Phenyl Carbocation

Here, angle strain for sp hybridization (Linear geometry) is much larger and therefore, destabilizes the phenyl carbocation. Hence, linear geometry is not possible in positively charged carbon of phenyl carbocation.

(2) Hybridization in Carbon = sp^{3-n}

Where, n = No. of pi bonds made by respective carbon

Fact- Pi bonds are never formed by hybridized orbitals, but are always formed by side-wise overlapping of unhybridized p-orbitals.

For example, for following compound-



The hybridization in different carbon atoms from left to right will be as under-



Here, (1) Single bond is always σ (sigma) bond

(2) Double bond consists of 1 σ and 1 π bonds

(3) Triple bond consists of 1 σ and 2 π bonds

(3) Determination of hybridization based on number of hybridized orbitals formed-

No. of hybridized orbitals formed

$$N = \frac{1}{2}(V + M + A - C)$$

Where, V = No. of valence electrons in central atom

M = No. of mono-valent atoms attached to the central atom

A = No. of charge on anion

C = No. of charge on cation

No. of hybridized orbitals formed

Type of Hybridization

2

sp

3

sp²

4

sp³

5

sp³d

6

sp³d²

7

sp³d³

Examples-

(1) For NH₃ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(5 + 3 + 0 - 0) \\ &= 4 \text{ (sp}^3\text{)} \end{aligned}$$

(2) For H₂O molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(6 + 2 + 0 - 0) \\ &= 4 \text{ (sp}^3\text{)} \end{aligned}$$

(3) For PCl₅ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(5 + 5 + 0 - 0) \\ &= 5 \text{ (sp}^3\text{d)} \end{aligned}$$

(4) For SF₄ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(6 + 4 + 0 - 0) \\ &= 5 \text{ (sp}^3\text{d)} \end{aligned}$$

(5) For SF₆ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(6 + 6 + 0 - 0) \\ &= 6 \text{ (sp}^3\text{d}^2\text{)} \end{aligned}$$

(6) For IF₇ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(7 + 7 + 0 - 0) \\ &= 7 \text{ (sp}^3\text{d}^3\text{)} \end{aligned}$$

(7) For ClF₃ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(7 + 3 + 0 - 0) \\ &= 5 \text{ (sp}^3\text{d)} \end{aligned}$$

(8) For ClF₅ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(7 + 5 + 0 - 0) \\ &= 6 \text{ (sp}^3\text{d}^2\text{)} \end{aligned}$$

(9) For XeF₂ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(8 + 2 + 0 - 0) \\ &= 5 \text{ (sp}^3\text{d)} \end{aligned}$$

(10) For XeF₄ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(8 + 4 + 0 - 0) \\ &= 6 \text{ (sp}^3\text{d}^2\text{)} \end{aligned}$$

(11) For XeF₆ molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(8 + 6 + 0 - 0) \\ &= 7 \text{ (sp}^3\text{d}^3\text{)} \end{aligned}$$

(12) For XeOF_2 molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(8 + 2 + 0 - 0) \\ &= 5 \text{ (sp}^3\text{d)} \end{aligned}$$

(13) For XeOF_4 molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(8 + 4 + 0 - 0) \\ &= 6 \text{ (sp}^3\text{d}^2\text{)} \end{aligned}$$

(14) For XeO_3 molecule-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(8 + 0 + 0 - 0) \\ &= 4 \text{ (sp}^3\text{)} \end{aligned}$$

(15) For H_3O^+ ion-

No. of hybridized orbitals formed,

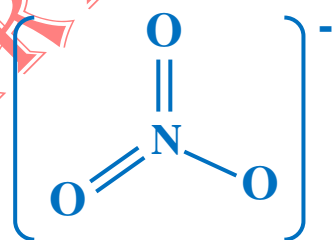
$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(6 + 3 + 0 - 1) \\ &= 4 \text{ (sp}^3\text{)} \end{aligned}$$

(16) For NH_4^+ ion-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(5 + 4 + 0 - 1) \\ &= 4 \text{ (sp}^3\text{)} \end{aligned}$$

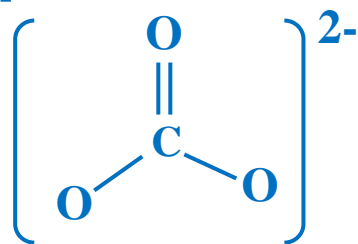
(17) For NO_3^- ion-



No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(5 + 0 + 1 - 0) \\ &= 3 \text{ (sp}^2\text{)} \end{aligned}$$

(18) For CO_3^{2-} ion-



No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(4 + 0 + 2 - 0) \\ &= 3 \text{ (sp}^2\text{)} \end{aligned}$$

(19) For NO_2^- ion-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(5 + 0 + 1 - 0) \\ &= 3 \text{ (sp}^2\text{)} \end{aligned}$$

(20) For NO_2^+ ion-

No. of hybridized orbitals formed,

$$\begin{aligned} N &= \frac{1}{2}(V + M + A - C) \\ &= \frac{1}{2}(5 + 0 + 0 - 1) \\ &= 2 \text{ (sp)} \end{aligned}$$

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