Prof. Linus Pauling (1931) first developed the Hybridization state theory in order to explain the structure of molecules such as methane (CH$_4$). This concept was developed for simple chemical systems but this one applied more widely later on and from today’s point of view it is considered an operative empirical for excusing the structures of organic and inorganic compounds along with their related problems. An innovative method proposed for the determination of hybridization state on time economic ground $^{2,3,4}$.

**Prediction of sp, sp$^2$, sp$^3$ Hybridization state**

We Know, hybridization is nothing but the mixing of orbital’s in different ratio to form some newly synthesized orbitals called hybrid orbitals. The mixing pattern is as follows:

- $s + p (1:1)$ - sp hybrid orbital; $s + p (1:2)$ - sp$^2$ hybrid orbital; $s + p (1:3)$ - sp$^3$ hybrid orbital

Formula used for the determination of sp, sp$^2$ and sp$^3$ hybridization state:

$$\text{Power on the Hybridization state of the central atom} = (\text{Total no of } \sigma \text{ bonds around each central atom} - 1)$$

All single (-) bonds are $\sigma$ bond, in double bond (=) there is one $\sigma$ and 1$\pi$, in triple bond (≡) there is one $\sigma$ and 2$\pi$. In addition to these each lone pair (LP) and Co-ordinate bond can be treated as one $\sigma$ bond subsequently.

**Eg.:**

a. In NH$_3$: central atom N is surrounded by three N-H single bonds i.e. three sigma ($\sigma$) bonds and one lone pair (LP) i.e. one additional $\sigma$ bond. So, in NH$_3$ there is a total of four $\sigma$ bonds [3 bond pairs (BPs) + 1 lone pair (LP)] around central atom N. Therefore, in this case power of the hybridization state of N = 4-1 = 3 i.e. hybridization state = sp$^3$.

b. In H$_2$O: central atom O is surrounded by two O-H single bonds i.e. two sigma ($\sigma$) bonds and two lone pairs i.e. two additional $\sigma$ bonds. So, altogether in H$_2$O there are four $\sigma$ bonds (2 bond pairs + 2 lone pairs) around central atom O, So, in this case power of the hybridization state of O = 4-1 =3 i.e. hybridization state of O in H$_2$O = sp$^3$.

c. In H$_3$BO$_3$: B has 3$\sigma$ bonds (3BPs but no LPs) and oxygen has 4$\sigma$ bonds (2BPs & 2LPs) so, in this case power of the hybridization state of B = 3-1 = 2 i.e. B is sp$^2$ hybridized in H$_3$BO$_3$. On the other hand, power of the hybridization state of O = 4-1= 3 i.e. hybridization state of O in H$_3$BO$_3$ is sp$^3$.

d. In I-Cl: I and Cl both have 4$\sigma$ bonds and 3LPs, so, in this case power of the hybridization state of both I and Cl = 4 - 1 = 3 i.e. hybridization state of I and Cl both are sp$^3$.

e. In CH$_2$=CH$_2$: each carbon is attached with 2 C-H single bonds (2 $\sigma$ bonds) and one C=C bond (1$\sigma$ bond), so, altogether there are 3 sigma bonds. So, in this case, power of the hybridization state of both C = 3-1 = 2 i.e. hybridization state of both C’s are sp$^2$. 
Prediction of sp$^3$d, sp$^3$d$^2$, and sp$^3$d$^3$ Hybridization States

In case of sp$^3$d, sp$^3$d$^2$, and sp$^3$d$^3$ hybridization state there is a common term sp$^3$ for which 4 sigma bonds are responsible. So, in addition to 4 sigma bonds, for each additional sigma, added one d orbital gradually as follows:-

- $5\sigma$ bonds = $4\sigma$ bonds + 1 additional $\sigma$ bond = sp$^3$d hybridization
- $6\sigma$ bonds = $4\sigma$ bonds + 2 additional $\sigma$ bonds = sp$^3$d$^2$ hybridization
- $7\sigma$ bonds = $4\sigma$ bonds + 3 additional $\sigma$ bonds = sp$^3$d$^3$ hybridization

Eg:-

a. IF$_4^+$: I has 7 e$^-$s in its outermost shell, so, in this case, subtract one e$^-$ from 7 i.e. 7 - 1 = 6. So, out of 6 electrons, 4 electrons form 4 I-F bonds i.e. 4 sigma bonds and there is one LP. So, altogether there are 5 $\sigma$ bonds. So, $5\sigma$ bonds = $4\sigma$ bonds + 1 additional $\sigma$ bond = sp$^3$d hybridization

b. IF$_7$: 7 I-F single bonds i.e. $7\sigma$ bonds = $4\sigma$ bonds + 3 additional $\sigma$ bonds = sp$^3$d$^3$ hybridization.

c. ICl$_2^-$: I has 7 e$^-$s in its outermost shell, so, in this case, add one e$^-$ with 7(overall charge on the compound) i.e. 07+1= 08. So, out of 08 electrons, 02 electrons form 02 I-Cl bonds i.e. 02 sigma bonds and there is 03 LPs. So, altogether there are 05$\sigma$ bonds. So, $5\sigma$ bonds = $4\sigma$ bonds + 01 additional $\sigma$ bond = sp$^3$d hybridization.

d. XeF$_4$: Xe, an inert gas, consider 8 e$^-$s in its outermost shell, 04 of which form 04 Xe-F sigma bonds and there is two LPs, i.e. altogether there is 06 $\sigma$ bonds = 04 $\sigma$ bonds + 02 additional $\sigma$ bonds = sp$^3$d$^2$ hybridization.

In case of determination of the hybridization state by using the above method, one must have a clear idea about the outermost electrons of different family members in the periodic table as follows:

<table>
<thead>
<tr>
<th>Family</th>
<th>Outermost electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen family</td>
<td>05</td>
</tr>
<tr>
<td>Oxygen family</td>
<td>06</td>
</tr>
<tr>
<td>Halogen family</td>
<td>07</td>
</tr>
<tr>
<td>Inert gas family</td>
<td>08</td>
</tr>
</tbody>
</table>

In case of cationic species you must remove requisite electron / electrons from the outermost orbit of the central atom and in case of anionic species you must add requisite electron with the outermost electrons of the central atom. Examples have been explored in Table 1.
Table 1: Total number of σ bonds and Hybridization State

<table>
<thead>
<tr>
<th>Total number of sigma (σ) bonds</th>
<th>Nature of Hybridization State</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>sp</td>
<td>BeCl₂, HgCl₂, C₂H₂, CO₂, CO, CdCl₂, ZnCl₂ etc.</td>
</tr>
<tr>
<td>3</td>
<td>sp²</td>
<td>BCl₃, AlCl₃, C₂H₄, C₆H₆, SO₂, SO₃, HNO₃, H₂CO₃, SnCl₂, PbCl₂ etc.</td>
</tr>
<tr>
<td>4</td>
<td>sp³</td>
<td>NH₄⁺, BF₄⁻, H₂SO₄, HClO₄, PCl₃, NCl₃, AsCl₃, HClO₃, ICl₂⁺, OF₂, HClO₂, SCl₂, HCIO, ICl, XeO₃ etc.</td>
</tr>
<tr>
<td>5</td>
<td>sp³d</td>
<td>PCl₅, SbCl₅, SF₄, ClF₃, BrF₃, XeF₂, ICl₂⁻ etc.</td>
</tr>
<tr>
<td>6</td>
<td>sp³d²</td>
<td>SF₆, AlF₆³⁻, SiF₆²⁻, PF₆⁻, IF₅, BrF₅, XeOF₄, XeF₄, BrF₄⁻, ICl₄⁻ etc.</td>
</tr>
<tr>
<td>7</td>
<td>sp³d³</td>
<td>IF₇, XeF₆ etc.</td>
</tr>
</tbody>
</table>

References


External Links

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