Jahn-Teller Theorem
**Jahn-Teller Theorem**

The Jahn-Teller Theorem was first published in 1937 named after Hermann Arthur Jahn and Edward Teller and it states that:

"any non-linear molecular system in a degenerate electronic state will be unstable and will undergo distortion to form a system of lower symmetry and lower energy thereby removing the degeneracy"

In above theorem we come across term electronic degeneracy, so what is electronic degeneracy?

An electronically degenerate state represents to the availability of more than one degenerate orbitals for an electron. Here the degenerate orbitals are asymmetrically occupied. E.g. d1 configuration in octahedral symmetry is said to be electronically degenerate since there are three t2g orbitals with same energy available for the electron to occupy.

```
  ↑  ↑  ↑
  XY XZ YZ
```

Electronically degenerate state of d1 configuration

Similarly, example of non-degenerate and symmetric orbital is d3 configuration in octahedral symmetry and that is because it is not possible to put two electrons in one orbital, which is against of Hund's rule of maximum multiplicity.

```
  ↑  ↑  ↑
  XY XZ YZ
```

Similarly, example of non-degenerate and symmetric orbital is d3 configuration in octahedral symmetry and that is because it is not possible to put two electrons in one orbital, which is against of Hund's rule of maximum multiplicity.
In the electronically degenerate state, if the orbitals are asymmetrically occupied, get more energy. Therefore, this system tries to get rid of this extra energy by lowering the overall symmetry of the molecule that is by undergoing distortion, which is known as **Jahn Teller distortion**.

Jahn Teller distortion is mostly observed in octahedral molecules. The Jahn Teller distortions depends on whether the orbital is filled asymmetrically or symmetrically and also whether it is t$_{2g}$ orbitals or eg orbital.

Now considering the fact that d$^3$, d$^8$, d$^{10}$, high spin d$^5$ and low spin d$^6$ are symmetrically distributed there is **no Jahn teller distortion** observed in these molecules.

<table>
<thead>
<tr>
<th>d$^3$ Configuration</th>
<th>d$^8$ Configuration</th>
<th>d$^{10}$ Configuration</th>
<th>d$^5$ (High Spin) Configuration</th>
<th>d$^6$ (Low Spin) Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\underline{\underline{x^2-y^2}}$ $z^2$</td>
<td>$\underline{\underline{x^2-y^2}}$ $z^2$</td>
<td>$\underline{\underline{x^2-y^2}}$ $z^2$</td>
<td>$\underline{\underline{x^2-y^2}}$ $z^2$</td>
<td>$\underline{\underline{x^2-y^2}}$ $z^2$</td>
</tr>
<tr>
<td>$\uparrow$ $\uparrow$ $\uparrow$</td>
<td>$\downarrow$ $\downarrow$ $\uparrow$</td>
<td>$\downarrow$ $\downarrow$ $\downarrow$ $\downarrow$</td>
<td>$\uparrow$ $\uparrow$ $\uparrow$</td>
<td>$\downarrow$ $\downarrow$ $\downarrow$ $\downarrow$</td>
</tr>
<tr>
<td>xy xz yz</td>
<td>xy xz yz</td>
<td>xy xz yz</td>
<td>xy xz yz</td>
<td>xy xz yz</td>
</tr>
</tbody>
</table>

When t$_{2g}$ orbitals are unevenly occupied, weak Jahn Teller distortions are observed, since very less energy is gained as t$_{2g}$ sets does not point directly at ligands.

Examples- d$^1$, d$^2$, low spin d$^4$ & d$^5$, high spin d$^6$ & d$^7$ configurations in octahedral environment
But when “eg” orbitals are unevenly occupied, strong Jahn Teller distortions are observed, since more energy is gained as “eg” orbitals are directly pointed to the ligands.

Examples- $d^9$, high spin $d^4$, low spin $d^7$ configuration in octahedral environment.
As we discussed above, the degeneracy of orbital’s can be removed by lowering the symmetry of molecule and this can be done either by octahedral elongation (Z-out distortion) or octahedral elongation (Z-in distortion).

\[ \text{Z-out distortion- In this type of distortion, the energies of d-orbital’s with z factor like } \text{dz}^2, \text{dxz, dyz are lowered by elongating the bonds along the z-axis. This is the most preferred distortion and occurs when the degeneracy occurs in eg level.} \]

Example \(d^4\) (high spin), \(d^7\) & \(d^8\) (Low spin), and \(d^9\) configuration in octahedral symmetry

Even though it is observed that Z-out distortion occurs mostly in eg level, theoretically it is impossible to predict type of distortion in eg level.

\[ \text{Z-in distortion- In this type of distortion, the energies of d-orbital’s with z factor like } \text{dz}^2, \text{dxz, dyz are increased by elongating the bonds along the z-axis.} \]
**Example- Octahedral d^1 configuration**

<table>
<thead>
<tr>
<th>Z- in distortion (Octahedral compression)</th>
<th>No distortion</th>
<th>Z- out distortion (Octahedral elongation)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Diagram" /></td>
<td><img src="image2.png" alt="Diagram" /></td>
<td><img src="image3.png" alt="Diagram" /></td>
</tr>
<tr>
<td><img src="image4.png" alt="Diagram" /></td>
<td><img src="image5.png" alt="Diagram" /></td>
<td><img src="image6.png" alt="Diagram" /></td>
</tr>
</tbody>
</table>

- \( z^2 \)
- \( x^2-y^2 \)
- \( xz \)
- \( yz \)
- \( xy \)

- \( x^2-y^2 \)
- \( z^2 \)
- \( xy \)
- \( xz \)
- \( yz \)

**Eg orbital’s**

**t_2g orbital’s**
Solved questions from NET, SET and Gate exams on Jahn Teller distortion

NET JUNE-2015

Among the complexes $K_4[Cr(CN)_6]$ (A), $K_4[Fe(CN)_6]$ (B), $K_3[Co(CN)_6]$ (C), $K_4[Mn(CN)_6]$ (D), Jahn teller distortion is expected in

1. A, B and C  
2. B, C and D  
3. A and D  
4. B and C

Ans) 3 , complex A and D

**Complex A** is $K_4[Cr(CN)_6]$ , the oxidation number on Cr = 4*charge on K+ x (Oxidation no. of Cr) +(charge on cyano group)*6 =0

\[4(1) + x(-1)6 = 0\]
\[4 + x - 6 = 0\]
\[x = 2\]

Therefore, Cr in +2 oxidation state

Outer electronic configuration of Chromium (Cr) is $4S^13d^5$

Outer electronic configuration of Cr $^{+2}$ is $3d^4$

CN ligand is strong field ligand and will result in low spin complex, therefore it is $d^4$ Low spin complex.
It (complex A) will have weak Jahn-Teller distortion due to asymmetric filled t_{2g} orbitals.

**Complex B** is K₄[Fe(CN)_6] where oxidation no. of Fe is +2.

Outer electronic configuration of Fe is 4s^2, 3d^6 and that of Fe^{+2} is 3d^6.

It is d^6 low spin complex.

Since t_{2g} orbital is symmetrically distributed, no Jahn-Teller distortion.

**Complex C** is K₃[Co(CN)_6] and the oxidation no. of Co in the complex is +3.

Outer electronic configuration of Co is 4s^2, 3d^7 and that of Co^{+3} is 3d^6.
It is d\(^6\) low spin complex because CN is strong field ligand and thus no Jahn Teller distortion as in case of complex B.

**Complex D** is \(K_4[Mn(CN)_6]\) and the oxidation state of Mn is +2

Outer electronic configuration of Mn is 4s\(^2\), 3d\(^5\) and that of Mn\(^{+2}\) is 3d\(^5\)

It is d\(^5\) low spin complex because CN is strong field ligand and has weak Jahn Teller distortion due to asymmetrically filled t\(_{2g}\) orbital.

\[
\begin{align*}
\text{d}^5 & \quad \text{(Low Spin)} \\
\text{Configuration} & \\
\end{align*}
\]

\[
\begin{align*}
\text{x}^2 - \text{y}^2 & \quad 2z^2 \\
\text{xy} & \quad \text{xz} \quad \text{yz} \\
\end{align*}
\]

**MHA SET-2018**

Jahn-Teller distortion will be exhibited by

(A) \([\text{Mn(H}_2\text{O)}_6]^{2+}\) \quad (B) \([\text{Cr(H}_2\text{O)}_6]^{3+}\)

(C) \([\text{Ni(H}_2\text{O)}_6]^{2+}\) \quad (D) \([\text{Cu(H}_2\text{O)}_6]^{2+}\)

Ans) D
Complex A is \([\text{Mn(H}_2\text{O)}_6]^{2+}\), oxidation state of Mn is +2 and the outer electron of \(\text{Mn}^{+2}\) is 3d\(^5\) and \(\text{H}_2\text{O}\) is weak field ligand resulting in high spin complex, therefore complex A is d\(^5\)(high spin complex).

\[
\text{d}^5 \quad (\text{Low Spin})
\]

\[
\text{Configuration}
\]

\[
\begin{array}{c}
\hline
x^2-y^2 \\
\hline
z^2
\end{array}
\]

\[
\hline
\hline
\end{array}
\]

\[
\begin{array}{l}
\uparrow \\
\uparrow \\
\downarrow
\end{array}
\]

\[
\begin{array}{lll}
xy & xz & yz
\end{array}
\]

No Jahn Teller distortion due to symmetrically filed t\(_2\)g and eg orbital’s.

Complex B is \([\text{Cr(H}_2\text{O)}_6]^{3+}\), oxidation state of Cr is +3 and the outer electron of \(\text{Cr}^{+3}\) is 3d\(^3\)

\[
\text{d}^3
\]

\[
\text{Configuration}
\]

\[
\begin{array}{c}
\hline
x^2-y^2 \\
\hline
z^2
\end{array}
\]

\[
\hline
\hline
\end{array}
\]

\[
\begin{array}{l}
\uparrow \\
\uparrow \\
\uparrow
\end{array}
\]

\[
\begin{array}{lll}
xy & xz & yz
\end{array}
\]

No Jahn Teller distortion due to symmetrically filed t\(_2\)g orbital’s.

Complex C is \([\text{Ni(H}_2\text{O)}_6]^{2+}\), oxidation state of Ni is +2 and the outer electron of \(\text{Ni}^{+2}\) is 3d\(^8\)
No Jahn Teller distortion due to symmetrically filled $t_{2g}$ and $e_g$ orbital’s

Complex D is $[\text{Cu(H}_2\text{O)}_6]^{2+}$, oxidation state of Cu is +2 and the outer electron of Cu$^{+2}$ is 3$d^9$

Complex D will exhibit strong Jahn teller distortion due to asymmetrically filled $e_g$ orbital’s

**IIT JAM-2017**

Jahn-Tadder distortion is/are observed in octahedral complexes with $d$-electron configuration of:
(A) d⁵-high spin  (B) d⁵-low spin  
(C) d⁶-high spin  (D) d⁶-low spin

Ans)  B and C

A is d⁵ high spin complex

\[ d^5 \text{ (High Spin)} \]
\[ \text{Configuration} \]

\[ \begin{array}{c}
\uparrow & \uparrow \\
\uparrow & \uparrow & \uparrow \\
x^2-y^2 & z^2 & xy & xz & yz \\
\end{array} \]

No Jahn Teller distortion due to symmetrically filed t_{2g} and eg orbital's

B is d⁵ low spin complex

\[ d^5 \text{ (Low Spin)} \]
\[ \text{Configuration} \]

\[ \begin{array}{c}
\downarrow & \downarrow \\
\uparrow & \uparrow & \uparrow \\
x^2-y^2 & z^2 & xy & xz & yz \\
\end{array} \]

Jahn Teller distortion due to asymmetrically filed t_{2g} orbital’s

C is d⁶ high spin complex.
d^6 (High Spin) Configuration

\[
\begin{array}{c}
\uparrow \uparrow \\
\downarrow \downarrow \\
\end{array}
\begin{array}{c}
x^2-y^2 \\
z^2 \\
xy \\
xz \\
yz \\
\end{array}
\]

Jahn Teller distortion due to asymmetrically filed t_2g orbital’s

D is d^6 low spin complex.

\[d^6\text{(Low Spin) Configuration}\]

\[
\begin{array}{c}
\downarrow \downarrow \downarrow \\
\end{array}
\begin{array}{c}
x^2-y^2 \\
z^2 \\
xy \\
xz \\
yz \\
\end{array}
\]

No Jahn Teller distortion due to symmetrically filed t_2g orbital’s
Thank you!