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A Smart Strategy for Prediction of Jahn-Teller Distortion in Octahedral Complexes

Shyam Sarkar

Assistant Professor, Department of Chemistry, Ananda Mohan College

Abstract

This article describes the prediction of Jahn-Teller distortion in a smarter way just like a dial number method for electronic configurations d^1 to d^{10} in the case of both high-spin (HS) and low-spin (LS) octahedral complexes of transition metal ions. These short tricks will help undergraduate chemistry students to solve problems associated with the prediction of Jahn-Teller distortion in the competitive examination, as it reduces the time in the exam hall. In addition, a few examples are explained based on smarter tricks for the prediction of Jahn-Teller distortion in octahedral complexes of transition metal ions.

Keywords: Crystal field theory, Jahn-Teller theorem, electron, degeneracy.

1. Introduction

In crystal field theory (CFT), the Jahn–Teller effect (JTE) which is also known as Jahn–Teller distortion (JTD), describes the geometrical distortion of non-linear molecules (or, ions) that is associated with some electron configurations. In the year of 1937, the effect was named after Hermann Arthur Jahn and Edward Teller, who first reported studies about the geometrical distortion of non-linear molecules [1]. The Jahn–Teller theorem states that "Any nonlinear molecular system in a degenerate electronic state will be unstable, and will undergo some sort of distortion to lower its symmetry and remove the degeneracy [2]. If more than one degenerate orbital is available for a single electron, then the state is called an electronically degenerate state. For example, in the d^1 electronic configuration, an electron may reside on any one of the three t_{2g} orbitals, hence it is said to be an electronically degenerate state. In an electronically degenerate state, electrons are asymmetrically distributed in orbitals and hence they will have more energy. Therefore, they will try to minimize their energy by lowering the overall symmetry of the molecule. This leads to the distortion in molecules, which is known as Jahn-Teller distortion.

2. Prediction of JTD in a conventional method

Prediction of the Jahn-Teller distortion (JTD) for octahedral complexes can be made in the following three ways by a conventional method which is shown in Table 1. A detailed distribution of electrons for electronic configurations d^1 to d^{10} in the case of both high-spin (HS) and low-spin (LS) octahedral complexes of transition metal ions is presented in Figure 1.

Table 1: Prediction of Jahn-Teller Distortion for different electronic configurations in octahedral complexes

Sl. No.	Types of Jahn-Teller Distortion	Configurations
1.	Strong Jahn-Teller distortion	$e_g \rightarrow$ asymmetrical

2.	Weak Jahn-Teller distortion	t_{2g} → asymmetrical
3.	No Jahn-Teller distortion	t_{2g}/e_g → symmetrical

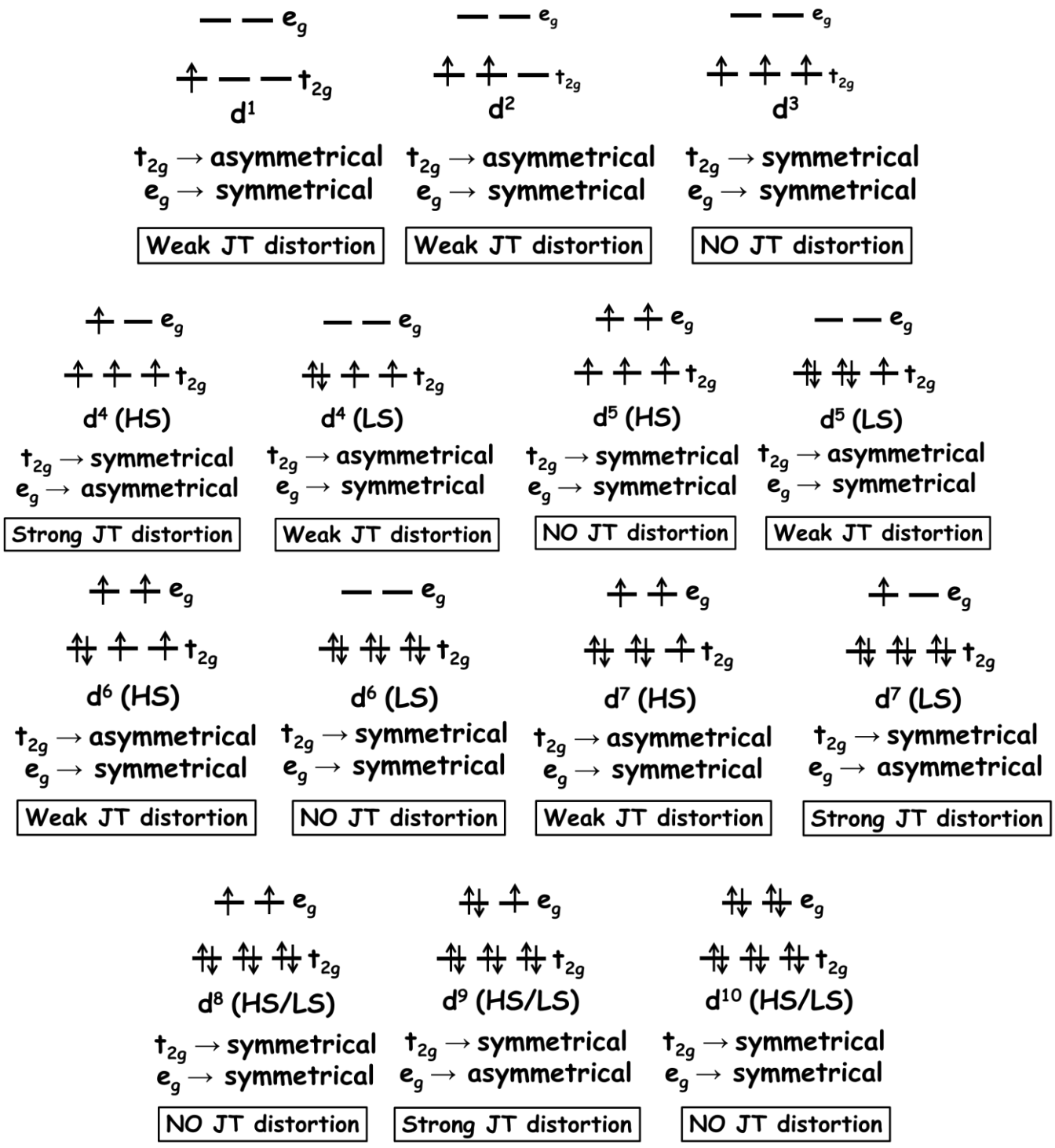

Figure 1: Schematic representation of prediction of the Jahn-Teller distortion for electronic configurations d^1 to d^{10} in an octahedral complex (both HS and LS) by a conventional method.

3. Prediction of JTD in modern method or just like a dial number method

Alternatively, the prediction of the Jahn-Teller distortion (JTD) for octahedral complexes can be made in a modern method just like a dial number as shown in Figure 2. Point 1 should be remembered as dial 49 for a high spin or dial 79 for a low spin octahedral complex. It means that d^4, d^9 in high spin and d^7, d^9 in low spin configurations will exhibit strong Jahn-Teller distortion. Similarly, point 2 should be remembered as dial 1267 for a high spin or dial 1245 for a low spin octahedral complex. It means that d^1, d^2, d^6, d^7 in high spin and d^1, d^2, d^4, d^5 in low spin configurations will exhibit weak Jahn-Teller distortion. Finally, point 3 should be remembered as dial 35810 for a high spin or dial 36810 for a low spin octahedral complex. It means that d^3, d^5, d^8, d^{10} in high spin and d^3, d^6, d^8, d^{10} in low spin configurations will not exhibit any Jahn-Teller distortion.

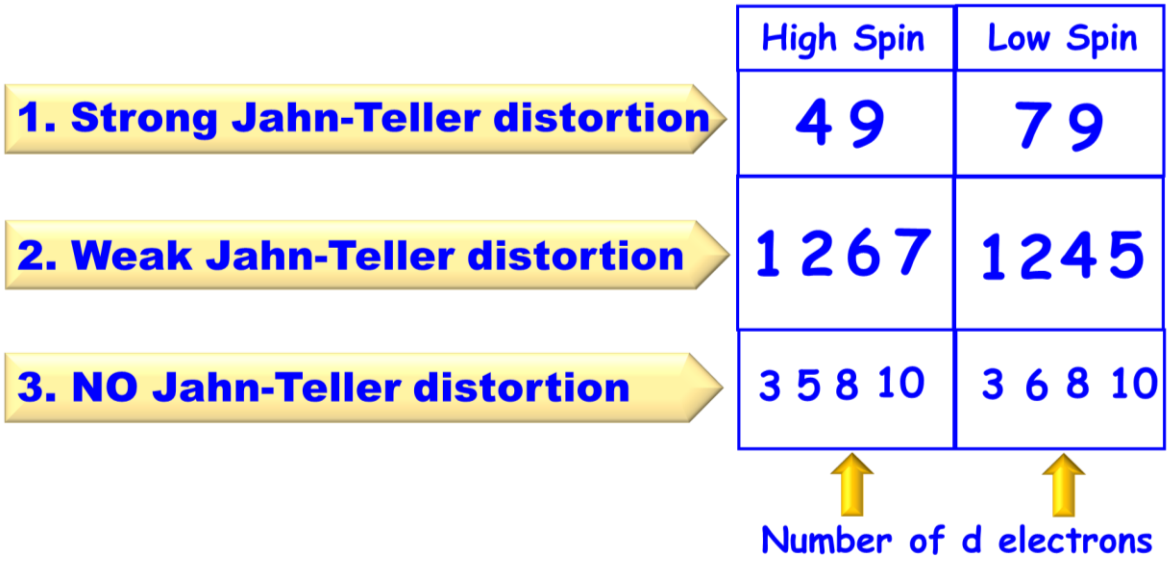

Figure 2: Schematic representation of prediction of the Jahn-Teller distortion for electronic configurations d^1 to d^{10} in an octahedral complex (both HS and LS) in a smarter way just like a dial number method.

4. Solved Problems

Example 1: Which one of the following configurations will show Jahn-Teller distortion in an octahedral field? [3]

(A) High spin d^8 (B) high spin d^4

(C) high spin d^5 (D) low spin d^6

Answer: If one can remember the scheme as shown in Figure 2, then it is quite easier to answer the problem within a few seconds. Hence, in a modern method or just like a dial number method, strong JTD is exhibited by high-spin d^4 electronic configuration as shown in point 1 of Figure 2. On the other hand, the rest given configurations i.e. d^8 (HS), d^5 (HS) and d^6 (LS) do not exhibit JTD as shown in point 3 of Figure 2.

Therefore, the correct answer is an option (B) high spin d^4.

Example 2: Which of the following complex ions would show strong Jahn-Teller distortion? [4]

(A) $[Cr(H_2O)_6]^{2+}$ (B) $[Ti(H_2O)_6]^{3+}$

(C) $[Co(H_2O)_6]^{2+}$ (D) $[Fe(H_2O)_6]^{2+}$

Answer: Similarly, if one can remember the scheme as shown in Figure 2, then it is quite easier to answer the problem within a few seconds. The electronic configuration of the given four transition metal ions is as follows:

$Cr^{2+} \rightarrow 3d^4$ (HS) → Strong JTD; $Ti^{3+} \rightarrow 3d^1$ → Weak JTD;

$Co^{2+} \rightarrow 3d^7$ (HS) → Weak JTD; $Fe^{2+} \rightarrow 3d^6$ (HS) → Weak JTD

Following the modern method or just like a dial number method, strong JTD is exhibited by Cr^{2+} ion, which has a high-spin d^4 electronic configuration as shown in point 1 of Figure 2. On the other hand, the rest given ions i.e. $Ti^{3+} \rightarrow d^1$, $Co^{2+} \rightarrow d^7$ (HS) and $Fe^{2+} \rightarrow d^6$ (HS) exhibit weak JTD as shown in point 2 of Figure 2.

Therefore, the correct answer is option (A) $[Cr(H_2O)_6]^{2+}$.

Example 3: For which one of the following metal ions, the strongest Jahn-Teller effect is observed in an octahedral field? [5]

(A) Ti^{3+} (B) V^{3+}

(C) Mn^{3+} (high spin) (D) Co^{3+} (high spin)

Answer: Similarly, if one can remember the scheme as shown in Figure 2, then it is quite easier to answer the problem within a few seconds. The electronic configuration of the given four transition metal ions is as follows:

$Ti^{3+} \rightarrow 3d^1$ → Weak JTD; $V^{3+} \rightarrow 3d^2$ → Weak JTD;

$Mn^{3+} \rightarrow 3d^4$ (HS) → Strong JTD; $Co^{3+} \rightarrow 3d^6$ (HS) → Weak JTD

Following the modern method or just like a dial number method, strong JTD is exhibited by Mn^{3+} (HS) ion, which has a d^4 electronic configuration as shown in point 1 of Figure 2. On the other hand, the rest given ions i.e. $Ti^{3+} \rightarrow d^1$, $V^{3+} \rightarrow d^2$ and $Co^{3+} \rightarrow d^6$ (HS) exhibit weak JTD as shown in point 2 of Figure 2.

Therefore, the correct answer is option (C) Mn^{3+} (high spin).

5. Conclusion

In conclusion, we have successfully demonstrated the smarter, quicker and more contemporary method for the prediction of Jahn-Teller distortion for electronic configurations d^1 to d^{10} in the case of both high-spin (HS) and low-spin (LS) octahedral complexes of transition metal ions. This article will help all undergraduate chemistry students to solve the problems that are related to the prediction of Jahn-Teller distortion in any type of examination within a few seconds. Students will also benefit from the explanation of three solved problems that are elaborately explained.

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