U.G. SEMESTER-IV

MJC-5 (T) : Inorganic Chemistry (s,p,d,f block elements)

Unit-1 : Periodic table and periodicity of elements
Topic : Slater's Rules (part-2)

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Examples of Applying Slater's Rules

Let's illustrate these rules with a few examples:

Example 1: Calculating Z_{eff} for a Valence Electron in Oxygen (O)

1. Electron Configuration: Oxygen ($Z = 8$) has the electron configuration: $1s^2 2s^2 2p^4$.
2. Group Arrangement: $(1s^2)(2s^2, 2p^4)$
3. Target Electron: We want to calculate Z_{eff} for a valence electron, so we choose one of the $2p$ electrons.
4. Calculate S:
    - Electrons in the same group $(2s^2, 2p^4)$: There are $(2-1) = 1$ other $2s$ electron and $(4-1) = 3$ other $2p$ electrons. Total = $1 + 3 = 4$ other electrons in the same group. Contribution: $4 \times 0.35 = 1.40$
    - Electrons in the $(n-1)$ group $(1s^2)$: There are 2 electrons in the $1s$ group. Contribution: $2 \times 0.85 = 1.70$
    - Electrons in $(n-2)$ and inner groups: None in this case.

Total $S = 1.40 + 1.70 = 3.10$

5. Calculate Z_{eff}: $Z_{eff} = Z - S = 8 - 3.10 = 4.90$

So, a valence electron in Oxygen experiences an effective nuclear charge of approximately 4.90. This is significantly less than the actual nuclear charge of 8, highlighting the shielding effect.

Example 2: Calculating Z_{eff} for a Valence Electron in Zinc (Zn)

1. Electron Configuration: Zinc ($Z = 30$) has the electron configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$.
2. Group Arrangement: $(1s^2)(2s^2, 2p^6)(3s^2, 3p^6)(3d^{10})(4s^2)$

3. Target Electron: We want to calculate Z_{eff} for a valence electron, so we choose one of the $4s$ electrons.
4. Calculate S:
   - Electrons in the same group ($4s^2$): There is 1 other $4s$ electron. Contribution: $1 \times 0.35 = 0.35$
   - Electrons in the $(n{-}1)$ group ($3s^2, 3p^6, 3d^{10}$): There are $2 + 6 + 10 = 18$ electrons in the $(n{-}1)$ shell ($3s, 3p, 3d$). Contribution: $18 \times 0.85 = 15.30$
   - Electrons in the $(n{-}2)$ group ($2s^2, 2p^6$): There are $2 + 6 = 8$ electrons in the $(n{-}2)$ shell ($2s, 2p$). Contribution: $8 \times 1.00 = 8.00$
   - Electrons in the $(n{-}3)$ group ($1s^2$): There are 2 electrons in the $(n{-}3)$ shell ($1s$). Contribution: $2 \times 1.00 = 2.00$

Total $S = 0.35 + 15.30 + 8.00 + 2.00 = 25.65$

5. Calculate Z_{eff}: $Z_{eff} = Z - S = 30 - 25.65 = 4.35$

The Z_{eff} for a $4s$ electron in Zinc is approximately 4.35.

Example 3: Calculating Z_{eff} for a $3d$ Electron in Zinc (Zn)

Let's calculate Z_{eff} for a $3d$ electron in Zinc, to show how the rules change for d-electrons.

1. Electron Configuration: $(1s^2)(2s^2, 2p^6)(3s^2, 3p^6)(3d^{10})(4s^2)$
2. Target Electron: One of the $3d$ electrons.
3. Calculate S:
   - Electrons in the group to the right ($4s^2$): These contribute 0.
   - Electrons in the same group ($3d^{10}$): There are $(10 - 1) = 9$ other $3d$ electrons. Contribution: $9 \times 0.35 = 3.15$
   - Electrons in the $(n{-}1)$ group ($3s^2, 3p^6$ for the $3d$ electron, $n = 3$): All electrons with principal quantum number less than n now contribute 1.00 because the target is a d electron. So all electrons in the $(n{-}1)$ shell are considered. There are $2 + 6 = 8$ electrons in the $3s, 3p$ shells. Contribution: $8 \times 1.00 = 8.00$
   - Electrons in the $(n{-}2)$ group ($2s^2, 2p^6$): There are $2 + 6 = 8$ electrons. Contribution: $8 \times 1.00 = 8.00$
   - Electrons in the $(n{-}3)$ group ($1s^2$): There are 2 electrons. Contribution: $2 \times 1.00 = 2.00$

Total $S = 3.15 + 8.00 + 8.00 + 2.00 = 21.15$

4. Calculate Z_{eff}: $Z_{eff} = Z - S = 30 - 21.15 = 8.85$

Notice that the Z_{eff} for a $3d$ electron (8.85) is significantly higher than for a $4s$ electron (4.35) in the same atom. This is because the $3d$ electrons are closer to the nucleus and less shielded than the $4s$ electrons by the inner shells. This difference in Z_{eff} helps explain why $3d$ electrons are often considered "inner" electrons in transition metals, even though their principal quantum number is lower than that of the $4s$ electrons which are removed first during ionization.

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