8.6.3: Applications of Tanabe-Sugano Diagrams

The Tanabe-Sugano diagrams can be used to interpret absorption spectra and gain insight into the properties of a coordination complex. For example, you could use the appropriate diagram to predict the number of transitions, assign the identity of a specific transition, or calculate the value of Δ for a specific metal complex.

How to use the Tanabe-Sugano Diagrams

1. Determine the d-electron count of the metal ion of interest.
2. Choose the appropriate Tanabe-Sugano diagram: this is the one matching the d-electron count of the metal ion. There is a full list of Tanabe-Sugano diagrams in the Resources Section.
3. Acquire an electronic spectrum of the metal complex and identify λ_{max} for spin-allowed (strong intensity) and spin forbidden (weak intensity) transitions.
4. Convert wavelength (λ_{max}) to energy (E) in wavenumbers (cm^{-1}) and generate energy ratios relative to the lowest-energy allowed transition. (i.e. $\frac{E_2}{E_1}$ and $\frac{E_3}{E_1}$).
5. Using a ruler, slide it across the printed Tanabe-Sugano diagram until the E/B ratios between lines is equivalent to the ratios found in step 4.
6. Solve for B using the E/B values (y-axis, step 4) and Δ_{oct}/B (x-axis, step 5) to yield the ligand field splitting energy, $Delta$ (Sometimes this is labeled as $10D_q$, and it is useful to know that $\Delta = 10D_q$).

Example 8.6.3.1: Chromium Splitting

A Cr^{3+} metal complex has strong transitions and λ_{max} at

- 431.03 nm,
- 781.25 nm, and
- 1,250 nm.

Determine the Δ_{oct} for this complex.

Solution

1. Cr has 6 electrons. Cr^{3+} has three electrons, so it has a d-configuration of d^3
2. Locate the d^3 Tanabe-Sugano diagram
3. Convert to wavenumbers:

$$\frac{10^7 (nm/cm)}{1250\ nm} = 8,000\ cm^{-1} \tag{8.6.3.1}$$

$$\frac{10^7 (nm/cm)}{781.25\ nm} = 13,600\ cm^{-1} \tag{8.6.3.2}$$

$$\frac{10^7 (nm/cm)}{431.03\ nm} = 23,200\ cm^{-1} \tag{8.6.3.3}$$

4. Allowed transitions are ${}^4T_{1g} \leftarrow {}^4A_{2g}$, ${}^4T_{1g} \leftarrow {}^4A_{2g}$ and ${}^4T_{2g} \leftarrow {}^4A_{2g}$.

Transition	Energy cm^{-1}	Ratios to lowest
${}^4T_{1g} \leftarrow {}^4A_{2g}$	23,200	2.9
${}^4T_{1g} \leftarrow {}^4A_{2g}$	13,600	1.7
${}^4T_{2g} \leftarrow {}^4A_{2g}$	8,000	1

5. Sliding the ruler perpendicular to the x-axis of the d^3 diagram yields the following values:

Δ_{oct}/B	10	20	30	40
Height E(v_3)/B	29	45	64	84

Δ_{oct}/B	10	20	30	40
Height $E(v_2)/B$	17	30	40	51
Height $E(v_1)/B$	10	20	30	40
Ratio $E(v_3)/E(v_1)$	2.9	2.25	2.13	2.1
Ratio $E(v_2)/E(v_1)$	1.7	1.5	1.33	1.275

6. Based on the two tables above it should be assessed that the Δ_{oct}/B value is 10. B is found by dividing E by the height.

Energy cm^{-1}	Height	B
23,200	29	800
13,600	17	800
8,000	10	800

7. Next multiply Δ_{oct}/B by B to yield the Δ_{oct} energy.

$$10 \times 800 = 8000\ cm^{-1} = \Delta_{oct} \tag{8.6.3.4}$$

Each problem is of varying complexity as several steps may be needed to find the correct Δ_{oct}/B values that yield the proper energy ratios.