

Understanding concepts related to light wavenumbers, particularly in the context of "cft" or crystallographic field theory. Let's break down some key points about light wavenumbers and their relevance to spectroscopy and crystallography:

## 1. Understanding Wavenumber

Definition:

- Wavenumber ( $\tilde{\nu}$ ) is a measure of the number of wave cycles per unit distance, and is typically used in spectroscopy to describe the frequency of light or electromagnetic radiation. It is the reciprocal of the wavelength ( $\lambda$ ) and is given by:

$$\tilde{\nu} = \frac{1}{\lambda}$$

- Wavenumber is commonly expressed in units of  $\text{cm}^{-1}$  (reciprocal centimeters).

Relation to Frequency and Energy:

- Wavenumber is directly proportional to frequency ( $\nu$ ) and energy ( $E$ ):

$$\tilde{\nu} = \frac{\nu}{c}$$

where  $c$  is the speed of light in a vacuum.

$$E = h\nu = hc\tilde{\nu}$$

where  $h$  is Planck's constant.

## 2. Crystallographic Field Theory (CFT) and Spectroscopy

### Crystallographic Field Theory (CFT):

- **Crystallographic Field Theory**, or more commonly **Crystal Field Theory (CFT)**, is used to describe the interaction between metal ions and the surrounding ligands in a coordination complex.

### Spectroscopy and Wavenumbers:

- In the context of spectroscopy, especially in UV-Vis (ultraviolet-visible) spectroscopy, wavenumbers are used to describe the energy levels of electronic transitions in molecules or ions.
- Crystal Field Theory helps explain the splitting of d-orbitals in metal complexes and the resulting electronic transitions that correspond to different wavenumbers.

## Key Concepts Related to Wavenumber in CFT:

- **Crystal Field Splitting Energy ( $\Delta_0$ ):** The energy difference between split d-orbitals in an octahedral or tetrahedral field. This can be related to the wavenumber of absorption or emission peaks observed in spectroscopy.
- **Transition Wavenumbers:** The wavenumbers corresponding to electronic transitions between the split d-orbitals. For example, in an octahedral complex, transitions between the  $t_{2g}$  and  $e_g$  orbitals can be observed in UV-Vis spectra.

## 3. Example Questions and How to Approach Them

### Example 1: Calculating Wavenumber from Energy

- **Question:** Given the energy of a transition is  $2.5 \times 10^{-19}$  Joules, calculate the wavenumber of the light associated with this transition.
- **Solution:**
  1. Convert the energy to wavenumber:

$$\tilde{\nu} = \frac{E}{hc}$$

2. Using Planck's constant  $h = 6.626 \times 10^{-34}$  J·s and the speed of light  $c = 3.00 \times 10^{10}$  cm/s, calculate:

$$\tilde{\nu} = \frac{2.5 \times 10^{-19}}{6.626 \times 10^{-34} \times 3.00 \times 10^{10}} \approx 1.25 \times 10^{15} \text{ cm}^{-1}$$

### Example 2: Interpreting Spectra

- **Question:** A UV-Vis spectrum shows a peak at  $15,000 \text{ cm}^{-1}$ . What is the energy associated with this peak?

- **Solution:**

1. Convert wavenumber to energy:

$$E = hc\tilde{\nu}$$

2. Using  $h = 6.626 \times 10^{-34}$  J·s and  $c = 3.00 \times 10^{10}$  cm/s:

$$E = 6.626 \times 10^{-34} \times 3.00 \times 10^{10} \times 15,000 \approx 2.98 \times 10^{-19} \text{ Joules}$$

### Summary

- **Wavenumber** is a key concept in spectroscopy, representing the frequency of light in reciprocal centimeters. It is inversely related to wavelength and directly related to the energy of electromagnetic radiation.
- **Crystal Field Theory** uses these concepts to explain how metal ions interact with ligands, resulting in different electronic transitions that can be observed and analyzed using spectroscopy.