

Engineering Chemistry – Unit 6 Premium Notes

Spectroscopic Techniques and Applications

RGPV Engineering Chemistry Notes

Unit Overview

This unit is one of the most important units in Engineering Chemistry because questions related to:

- Spectroscopy
- Electronic Spectroscopy
- Vibrational Spectroscopy
- Rotational Spectroscopy
- Instrumentation
- Applications of Spectroscopy

are frequently asked in RGPV examinations.

This unit is important for:

- Semester Exams
 - Viva Questions
 - Competitive Exams
 - Research Applications
 - Industrial Analysis
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Introduction to Spectroscopy

Definition

Spectroscopy is the study of interaction between electromagnetic radiation and matter.

When electromagnetic radiation falls on matter, absorption or emission of energy takes place.

This helps in studying:

- structure of molecules
- bonding

- energy levels
 - chemical composition
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Electromagnetic Spectrum

The electromagnetic spectrum consists of different radiations arranged according to wavelength.

Main regions are:

- Gamma rays
 - X-rays
 - Ultraviolet rays
 - Visible light
 - Infrared rays
 - Microwave
 - Radio waves
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Basic Principle of Spectroscopy

Principle

Atoms and molecules absorb energy only at specific wavelengths.

When energy is absorbed:

- electrons move to higher energy levels
- molecular vibrations increase
- molecular rotations occur

This absorbed energy is measured using spectroscopic instruments.

Terms Used in Spectroscopy

1. Wavelength

Distance between two consecutive waves.

Symbol:

λ

2. Frequency

Number of waves passing through a point per second.

Symbol:

ν

3. Wave Number

Reciprocal of wavelength.

Symbol:

$\tilde{\nu}$

Formula:

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

4. Intensity

Amount of absorbed or emitted radiation.

Instrumentation of Spectroscopy

Basic parts of spectroscopic instruments are:

1. Radiation Source
 2. Monochromator
 3. Sample Holder
 4. Detector
 5. Recorder
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1. Radiation Source

Provides electromagnetic radiation.

Examples:

- Tungsten lamp
 - Hydrogen lamp
 - Mercury lamp
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2. Monochromator

Separates light into different wavelengths.

3. Sample Holder

Contains sample to be analyzed.

4. Detector

Detects absorbed radiation.

5. Recorder

Displays obtained spectrum.

Applications of Spectroscopy

Spectroscopy is widely used in:

- Chemical analysis
- Structure determination
- Medical diagnosis
- Drug analysis
- Pollution monitoring

- Research laboratories
 - Food industries
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Electronic Spectroscopy

Definition

Electronic spectroscopy studies transitions of electrons from lower energy level to higher energy level.

It mainly involves:

- UV spectroscopy
 - Visible spectroscopy
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Principle of Electronic Spectroscopy

When molecules absorb UV or visible radiation:

Electrons jump from lower energy orbital to higher energy orbital.

Types of Electronic Transitions

1. $\sigma \rightarrow \sigma^*$ Transition

Electron moves from sigma bonding orbital to antibonding orbital.

Requires high energy.

2. $n \rightarrow \sigma^*$ Transition

Non-bonding electron moves to antibonding orbital.

3. $\pi \rightarrow \pi^*$ Transition

Pi electrons move to antibonding orbital.

Common in organic compounds.

4. $n \rightarrow \pi^*$ Transition

Non-bonding electron moves to pi antibonding orbital.

Instrumentation of UV-Visible Spectroscopy

Main parts:

- Radiation source
 - Monochromator
 - Sample cell
 - Detector
 - Recorder
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Applications of Electronic Spectroscopy

- Identification of compounds
 - Determination of concentration
 - Detection of impurities
 - Analysis of organic compounds
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Vibrational Spectroscopy

Definition

Vibrational spectroscopy studies vibration of molecules.

Mainly involves:

Infrared (IR) spectroscopy.

Principle of Vibrational Spectroscopy

When IR radiation is absorbed:

Molecules vibrate continuously.

Types of vibrations:

- Stretching vibration
 - Bending vibration
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1. Stretching Vibrations

Bond length changes.

Types:

- Symmetric stretching
 - Asymmetric stretching
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2. Bending Vibrations

Bond angle changes.

Characteristics of IR Spectroscopy

- Used for functional group analysis
 - Useful for organic compounds
 - Gives molecular structure information
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Applications of Vibrational Spectroscopy

- Identification of functional groups
 - Structure analysis
 - Pharmaceutical analysis
 - Polymer analysis
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Rotational Spectroscopy

Definition

Rotational spectroscopy studies rotational motion of molecules.

Mainly observed in microwave region.

Principle of Rotational Spectroscopy

When microwave radiation is absorbed:

Molecules rotate around their axis.

Conditions for Rotational Spectroscopy

- Molecule should have permanent dipole moment
 - Molecule should rotate freely
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Rotational Spectrum of Diatomic Molecules

Diatomic molecules contain two atoms.

Examples:

- HCl
 - CO
 - NO
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Characteristics of Rotational Spectra

- Equally spaced lines obtained
 - Useful for bond length determination
 - Gives molecular structure information
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Applications of Rotational Spectroscopy

- Determination of bond length
 - Molecular structure analysis
 - Gas phase analysis
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Difference Between Electronic, Vibrational and Rotational Spectroscopy

Electronic Spectroscopy	Vibrational Spectroscopy	Rotational Spectroscopy
Studies electronic transitions	Studies molecular vibrations	Studies molecular rotations
UV-visible region	Infrared region	Microwave region
High energy	Medium energy	Low energy
Used in compound analysis	Used for functional groups	Used for molecular structure

Advantages of Spectroscopy

- Accurate analysis
 - Fast process
 - Non-destructive method
 - Highly sensitive
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Limitations of Spectroscopy

- Expensive instruments
 - Skilled operation required
 - Complex spectra interpretation
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Numerical Concept – Wave Number

Formula

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

Example

If wavelength:

$$\lambda = 5 \times 10^{-4} \text{ cm}$$

Find wave number.

Solution

$$\tilde{\nu} = 1 / (5 \times 10^{-4})$$

$$\tilde{\nu} = 2000 \text{ cm}^{-1}$$

Final Answer

Wave number = 2000 cm^{-1}

Most Important 14 Marks Questions

1. Explain principle and instrumentation of spectroscopy.
2. Explain electronic spectroscopy.
3. Explain UV-visible spectroscopy.
4. Explain vibrational spectroscopy.
5. Explain IR spectroscopy.
6. Explain rotational spectroscopy.
7. Explain rotational spectroscopy of diatomic molecules.
8. Differentiate electronic, vibrational and rotational spectroscopy.
9. Explain applications of spectroscopy.
10. Numerical problems based on wave number.

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Detailed 14 Marks Important Questions with Answers
