Government PG College, Ambala Cantt.

Course file: Session 2023-24

Faculty Name: Dr. ABHA CHAUDHARY

Class: B. Sc. /Semester V

Subject Code and name: Paper-XIX (CH-305)/Physical Chemistry

Syllabus

M.Marks: 40 **External: 32 Internal: 8**

Time: 3 Hrs.

Note: Nine questions will be set. **Q.No.1**, based on whole syllabus, is compulsory. There will be four questions from section **A** and four from section **B**. Candidates will be required to attempt five questions in all, selecting at least two questions from each section. Question no.1 carry 8 marks and all questions in Section A & B (not more than 2-3 parts) carry 6 marks each**.**

Section-A

Quantum Mechanics-I: Black-body radiation, Plank's radiation law, photoelectric effect, postulates of quantum mechanics, quantum mechanical operator s, commutation relations, Hamiltonian operator, Hermi tian operator, average value of square of Hermitian as a positive quantity, Role of operators in quantum mechanics, To show quantum mechanically that position and momentum cannot be predicated simul taneously, Determination of wave function & energy of a particle in one dimensional box.

Physical Proper ties and Molecular Structure: Optical activity, polarization – (Clausius – Mossotti equation derivation excluded). Orientation of dipoles in an electric field, dipole moment, induced dipole moment, measurement of dipole moment -temperature method and refractivity method, dipole moment and structure of molecules, Magnetic permeability, magnetic susceptibility and its de termination. Applicat ion of magnetic susceptibility, magnetic properties – paramagnetism, diamagnetism and ferromagnetism.

Section-B

Spectroscopy: Introduction: Electromagnetic radiation, regions of spectrum, basic features of spectroscopy, statement of Born-oppenheimer approximation, Degrees of freedom.

Rotational Spectrum

Selection rules, Energy levels of rigid rotator (semi-classical principles), rotational spectra of diatomic molecules , spectral intensity distribution using population distribution (Maxwell-Boltzmann distribution), determination of bond length and isotopic effect.

Vibrational spectrum

Selection rules, Energy levels of simple harmonic oscillator, pure vibrational spectrum of diatomic molecules, determination of force constant and qualitative relation of force constant and bond energy, idea of vibrational frequencies of different functional groups.

Raman Spectrum

Concept of polarizibility, pure rotational and pure vibrational Raman spectra of diatomic molecules, selection rules, Quantum theory of Raman spectra.

Give more stress on numerical problems of all spectroscopy.

Text Books

1. Physical Chemistry, Modern's Publications
2. Physical Chemistry, Pradeep's Publications
3. R Chand, Physical chemistry, Semester V

Reference Books

1. B. R. Puri, Madan S. Pathania , L. R. Sharma *Principles of Physical Chemistry, 48th Ed.,* Vishal Publications.
2. Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).

COURSE OBJECTIVES

The course objectives outlined are as follows:

Quantum Mechanics-I: Identify Black-body radiation, Derive Plank's radiation law, Analyse photoelectric effect, Understand quantum mechanics, quantum mechanical operator s, commutation relations, Hamiltonian operator, Hermitian operator, Find out the average value of square of Hermitian as a positive quantity, Identify Role of operators in quantum mechanics, Show quantum mechanically that position and momentum cannot be predicated simultaneously, Determine the wave function & energy of a particle in one dimensional box.

Physical Properties and Molecular Structure: Understand Optical activity and polarization – Write Clausius – Mossotti equation, Study the orientation of dipoles in an electric field, dipole moment, induced dipole moment, Measurement of dipole moment by temperature method and refractivity method, dipole moment and structure of molecules, Determine Magnetic permeability, and magnetic susceptibility. Apply magnetic susceptibility, differentiate between paramagnetism, diamagnetism and ferromagnetism.

Spectroscopy: Introduce Electromagnetic radiation, Analyse the regions of spectrum, Identify basic features of spectroscopy, State Born-oppenheimer approximation, Calculate Degrees of freedom.

Rotational Spectrum

Explain Selection rules, Derive the Energy of rigid rotator, understand the rotational spectra of diatomic molecule, Identify spectral intensity distribution using population distribution (Maxwell-Boltzmann distribution), Determine the bond length and isotopic effect

Vibrational spectrum

Derive the energy of simple harmonic oscillator, pure vibrational spectrum of diatomic molecules, Determine the force constant and qualitative relation of force constant and bond energy, Understand the idea of vibrational frequencies of different functional groups.

Raman Spectrum

Understand the concept of polarizibility, differentiate between the pure rotational and pure vibrational Raman spectra of diatomic molecules, Identify selection rules, Explain Quantum theory of Raman spectra.

COURSE OUTCOMES

After completing this course, the learner will be able to:

1. To know about dual characteristic of matter and extend this fact to obtain postulates of quantum mechanics and quantum-mechanical operators, apply Schrödinger equation to determine the physical observables for particle in a box.
2. To be able to explain about the physical and magnetic properties associated with various molecular substances
3. To have sound knowledge about the consequences of interaction of radiation with matter resulting into various types of spectra.
4. To be able to solve various numerical problems related to spectroscopy.

Lesson Plan

Week No	Scheduled Dates	Topics to be covered
1	24-29 July	**Physical Proper ties and Molecular Structure** Optical activity, polarization – (Clausius – Mossotti equation derivation excluded). Orientation of dipoles in an electric field, dipole moment,
2	31 July- 5 August	Induced dipole moment, measurement of dipole moment - temperature method and refractivity method,
3	7-12 August	dipole moment and structure of molecules, Magnetic permeability, magnetic susceptibility and its de termination.
4	14-19 August	Application of magnetic susceptibility, magnetic properties – paramagnetism, diamagnetism and ferromagnetism
5	21-26 August	**Spectroscopy:** Introduction: Electromagnetic radiation, regions of spectrum, basic features of spectroscopy, statement of Born-oppenheimer approximation
6	28 August - 2 September	Degrees of freedom. **Rotational Spectrum:** Selection rules, Energy levels of rigid rotator (semi-classical principles), rotational spectra of diatomic molecules
7	4-9 September	spectral intensity distribution using population distribution (Maxwell-Boltzmann distribution), determination of bond length and isotopic effect
8	11-16 September	**Vibrational spectrum** Selection rules, Energy levels of simple harmonic oscillator, pure vibrational spectrum of diatomic molecules
9	18-23 September	determination of force constant and qualitative relation of force constant and bond energy, idea of vibrational frequencies of different functional groups **Raman Spectrum:** Concept of polarizibility,
10	25-30 September	pure rotational and pure vibrational Raman spectra of diatomic molecules, selection rules, Quantum theory of Raman spectra.
11	2-7 October	**Quantum Mechanics-I** Black-body radiation, Plank's radiation law, photoelectric effect, postulates of quantum mechanics
12	9-14 October	quantum mechanical operators, commutation relations,
13	16-21 October	Hamiltonian operator, Hermitian operator, average value of square of Hermitian as a positive quantity,
14	23-28 October	Role of operators in quantum mechanics, To show quantum mechanically that position and momentum cannot be predicated simultaneously,
15	30 October - 4 November	Determination of wave function & energy of a particle in one dimensional box.
16	13-18 November	Revision

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