



Jyoti Nivas College Autonomous
Hosur Road, Koramangala, Bangalore – 560095
Department of Chemistry
Programme: B. Sc.
V Semester
Chemistry – VI NEP
Advanced Physical Chemistry and Spectroscopy I

CREDITS:4

NO. OF HOURS: 60

Course Code: 21VCH6T

Course Objectives: This course aims to impart to the student, knowledge of:

I. Understanding Core Concepts:

1. A comprehensive understanding of advanced topics in physical chemistry including chemical kinetics, photochemistry, electrochemistry, and quantum mechanics.
2. Principles and theories underlying various spectroscopic techniques such as rotational, vibrational, Raman, electronic, and NMR spectroscopy.

II. Analytical Skills:

3. Theoretical models and mathematical equations to analyze and predict the behaviour of chemical systems.
4. Problem-solving skills through the application of kinetic, thermodynamic, and quantum mechanical principles to real-world scenarios.
5. Quantitative analysis and interpretation of experimental data related to reaction rates, electrochemical cells, and spectroscopic measurements.

III. Practical Applications:

6. Chemical kinetics to understand and control reaction mechanisms and rates in industrial and research settings.
7. Photochemical principles in practical applications such as photochemical synthesis, photobiology, and materials science.
8. Electrochemical concepts in designing and analyzing batteries, fuel cells, and electrochemical sensors.
9. Quantum mechanical methods in computational chemistry to model and predict molecular behaviour.
10. Spectroscopic techniques for the identification and characterization of chemical substances in various fields including pharmaceuticals, environmental science, and materials research.

IV. Critical Thinking:

11. Scientific literature and data to draw informed conclusions about chemical phenomena.

12. Designing and conducting experiments, as well as to analyze and interpret the resulting data.
13. The limitations and assumptions inherent in different theoretical approaches and experimental methods.
14. Integrating various sub-disciplines of chemistry to address complex chemical problems.

Course Specific Outcomes:

After the completion of this course, the student would be able to:

I. Understand Core Concepts:

- CO1. Gain a comprehensive understanding of advanced topics in physical chemistry including chemical kinetics, photochemistry, electrochemistry, and quantum mechanics.
- CO2. Understand the principles and theories underlying various spectroscopic techniques such as rotational, vibrational, Raman, electronic, and NMR spectroscopy.

II. Showcase Analytical Skills:

- CO3. Develop the ability to apply theoretical models and mathematical equations to analyze and predict the behavior of chemical systems.
- CO4. Enhance problem-solving skills through the application of kinetic, thermodynamic, and quantum mechanical principles to real-world scenarios.
- CO5. Perform quantitative analysis and interpretation of experimental data related to reaction rates, electrochemical cells, and spectroscopic measurements.

III. Possess Practical Applications:

- CO6. Apply knowledge of chemical kinetics to understand and control reaction mechanisms and rates in industrial and research settings.
- CO7. Utilize photochemical principles in practical applications such as photochemical synthesis, photobiology, and materials science.
- CO8. Use electrochemical concepts in designing and analyzing batteries, fuel cells, and electrochemical sensors.
- CO9. Implement quantum mechanical methods in computational chemistry to model and predict molecular behaviour.
- CO10. Employ spectroscopic techniques for the identification and characterization of chemical substances in various fields including pharmaceuticals, environmental science, and materials research.

IV. Develop Critical Thinking:

- CO11. Critically evaluate scientific literature and data to draw informed conclusions about chemical phenomena.
- CO12. Develop the ability to design and conduct experiments, as well as to analyze and interpret the resulting data.
- CO13. Foster a deeper understanding of the limitations and assumptions inherent in different theoretical approaches and experimental methods.
- CO14. Encourage the integration of knowledge from various sub-disciplines of chemistry to address complex chemical problems.

CO No.	Course outcomes statement	Knowledge level
1.	Gain a comprehensive understanding of advanced topics in physical chemistry including chemical kinetics, photochemistry, electrochemistry, and	K1, K2, K3

	quantum mechanics.	
2.	Understand the principles and theories underlying various spectroscopic techniques such as rotational, vibrational, Raman, electronic, and NMR spectroscopy.	K1, K2, K3
3.	Develop the ability to apply theoretical models and mathematical equations to analyze and predict the behaviour of chemical systems.	K1, K2, K3
4.	Enhance problem-solving skills through the application of kinetic, thermodynamic, and quantum mechanical principles to real-world scenarios.	K1, K2, K3
5.	Perform quantitative analysis and interpretation of experimental data related to reaction rates, electrochemical cells, and spectroscopic measurements.	K1, K2, K3, K4
6.	Apply knowledge of chemical kinetics to understand and control reaction mechanisms and rates in industrial and research settings.	K1, K2, K3
7.	Utilize photochemical principles in practical applications such as photochemical synthesis, photobiology, and materials science.	K1, K2, K3
8.	Use electrochemical concepts in designing and analyzing batteries, fuel cells, and electrochemical sensors.	K1, K2, K3
9.	Implement quantum mechanical methods in computational chemistry to model and predict molecular behaviour.	K1, K2, K3
10.	Employ spectroscopic techniques for the identification and characterization of chemical substances in various fields including pharmaceuticals, environmental science, and materials research.	K1, K2, K3
11.	Critically evaluate scientific literature and data to draw informed conclusions about chemical phenomena.	K1, K2, K3, K4, K5
12.	Develop the ability to design and conduct experiments, as well as to analyze and interpret the resulting data.	K1, K2, K3, K4, K5, K6
13.	Foster a deeper understanding of the limitations and assumptions inherent in different theoretical approaches and experimental methods.	K1, K2, K3, K4
14.	Encourage the integration of knowledge from various sub-disciplines of chemistry to address complex chemical problems.	K1, K2, K3, K4, K5, K6

K1 – Remember, K2 – Understand, K3 – Apply, K4 – Analyze, K5 – Evaluate, K6 – Create

Mapping of COs with POs

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	✓									✓
CO 2	✓									✓
CO 3	✓	✓		✓					✓	✓
CO 4	✓	✓		✓					✓	✓
CO 5	✓	✓		✓			✓		✓	✓
CO 6	✓	✓		✓			✓		✓	✓
CO 7	✓	✓		✓			✓		✓	✓
CO 8	✓	✓		✓			✓		✓	✓
CO 9	✓	✓		✓			✓		✓	✓
CO 10	✓	✓		✓			✓		✓	✓
CO 11	✓	✓		✓			✓		✓	✓
CO 12	✓	✓		✓	✓		✓		✓	✓
CO 13	✓	✓		✓			✓		✓	✓
CO14	✓	✓		✓			✓		✓	✓

Programme Objectives aligned with Graduate attributes

PO1- Knowledge

PO2- Scientific thinking

PO3- Entrepreneurial skills

PO4- Analytical skills

PO5- Communication skills

PO6- Social commitment

PO7- Research and Inquiry

PO8- Conservation of Environment

PO9- Employability

PO10- Academic orientation

Syllabus

Paper VI: Advanced Physical Chemistry and Spectroscopy I **60 Hours**

Unit I **15 Hours**

Chemical Kinetics **10 Hours**

Macroscopic and microscopic kinetics. Review of theories of reaction rate- collision theory and transition state theory. Comparison of collision theory with transition state theory. Arrhenius equation- characteristics. Significance of energy of activation, temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wynne-Jones and Eyring treatment), reaction between ions in solutions - Influence of ionic strength on reaction rates (primary and secondary salt effects). Numerical problems. Concept of Steady-state kinetics: Chain reactions - chain length and chain inhibition, comparison of photochemical and thermal reaction of hydrogen and bromine.

Photochemistry **5 Hours**

Laws of photochemistry (Grotthus-Draper and Stark-Einstein laws). Quantum yield (definition, Einstein and its significance). Actinometry (explain uranyl oxalate actinometer for measurement of the energy of radiation absorbed). Examples of low and high quantum yields (examples for $\phi = 1$, $\phi < 1$ and ϕ very high): Photochemical combination of H_2 and Cl_2 . Photochemical equilibrium (statement). Photosensitized reactions (explanation taking example), quenching (explanation taking example). Singlet and triplet states. Fluorescence and phosphorescence (explanation using Jablonski diagram). Role of photochemical reactions in biochemical processes (bioluminescence), photo stationary states, chemiluminescence (definition and with example).

Unit II **15 Hours**

Electrochemistry II **9 Hours**

Reversible and irreversible cells (definition and examples. Introduction of an electrochemical cell and explanation taking suitable examples). Concept of EMF of a cell (origin of EMF in an electrochemical cell, oxidation and reduction reactions, single electrode potential, reduction and oxidation potentials and formula for EMF). Measurement of EMF of a cell (compensation method, mention of standard cell-Weston cadmium cell). Nernst equation (derivation from free energy concepts for a cell and then for a single electrode) and its importance. Numerical problems. Types of electrodes [examples and their applications (i) metal/metal ion electrode - Zn/Zn^{2+} and Cu/Cu^{2+} ; (ii) metal/insoluble salt/anion electrode-calomel and $Ag/AgCl$ electrodes; (iii) metal/gas-ion electrode- hydrogen electrode; (iv) inert metal/ organic compound electrode- quinhydrone electrode; (v) Glass electrode and (vi) Red-ox electrode]. Standard electrode potential (definition, explanation of the importance of electrodes. Mention of primary-SHE and secondary reference electrodes -calomel electrode, convention of representing a cell, differences between standard reduction potential and standard oxidation potential). Electrochemical series and its applications (definition, standard reduction potential, SRP values of common reference electrodes, uses). Thermodynamics of a reversible cell (equations depicting the relationship between free energy change, enthalpy change, entropy change, equilibrium constant and EMF). Calculation of thermodynamic properties: ΔG , ΔH

and ΔS from EMF data. Numerical problems. Calculation of equilibrium constant from EMF data (Numerical problems). Concentration cells with transference and without transference (definition and examples). Liquid junction potential (definition) and salt bridge (significance). pH determination using hydrogen electrode, Glass and quinhydrone electrodes (setting up of a suitable electrochemical cell, measuring EMF and calculating pH). Numerical problems.

Quantum Mechanics II

6 Hours

Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermitian operators. Angular Momentum operators and their properties. Commutation of operators. Solutions of Schrödinger wave equation for a particle in a three-dimensional box (no derivation). Quantum mechanical degeneracy, tunnelling (no derivation). Application of Schrödinger equation to harmonic oscillator (Equations to be assumed) and rigid rotator (with derivation). Eigenfunctions and eigenvalues of angular momentum. Ladder operator method for angular momentum. Solutions to Schrödinger equation in spherical polar coordinates (no derivation). Θ , Φ and R equations. Total wave functions of a hydrogen atom. Quantum numbers and their characteristics.

Unit III

15 Hours

Introduction to Spectroscopy

1 Hour

Interaction of electromagnetic radiation with molecules (emission and absorption spectra, electromagnetic spectrum in terms of wavelength/wave number, difference between atomic and molecular spectra and molecular energy levels) and various types of spectra (UV, IR, MW, Raman, and NMR and mention of the region), Born - Oppenheimer approximation (statement and explanation).

Rotational Spectroscopy

4 Hours

Expressions for energy of diatomic rigid rotor in terms of joule and m^{-1} , rotational constant, reduced mass, moment of inertia and spacing between rotational levels. Selection rules (statement, expression for frequency for transition between J to $(J+1)$, condition for absorption and spacing between spectral lines), intensities of spectral lines, determination of bond lengths of diatomic molecules. Numerical problems.

Vibrational Spectroscopy

8 Hours

Classical equation of vibration (mention of expression for frequency/wave number for diatomic (S H O), computation of force constant (definition of force constant, significance and statement of Hooke's law) amplitude of diatomic molecular vibrations (potential energy curve for diatomic SHO, expression for vibrational energy (from solutions to Schrödinger wave equation), zero point energy, selection rule, condition for absorption and fundamental vibrational frequency). Anharmonicity (difference in potential energy curves for SHO and others), Morse potential (energy expression for anharmonic oscillator, selection rules), dissociation energies, fundamental frequencies, overtones (compare the intensities), hot bands, degrees of freedom for polyatomic molecules (linear and non-linear – explanation taking suitable examples), modes of vibration (stretching and bending vibrations – types, comparison of frequencies, sketching of vibrational modes for CO_2 and H_2O), concept of group frequencies. Vibration-rotation spectroscopy – (pure vibrational spectra in liquids and mixing of vibration

and rotational levels) diatomic vibrating rotator (expression for energy, selection rule and expression for energy change), P, Q, R branches explanation using diagram.

Raman Spectroscopy

2 Hours

Raman scattering, Rayleigh scattering, polarizability and Raman shift Qualitative treatment of rotational Raman effect (selection rule, expression for energy difference of a rigid diatomic rotor); Vibrational Raman spectra (selection rule) Stokes and anti-Stokes lines (explanation using diagram); their intensity difference, Comparison between Raman and IR spectroscopy, rule of mutual exclusion (explanation using CO₂).

Unit IV

15 Hours

Electronic Spectroscopy

5 Hours

(Complexity of electronic spectra), Franck-Condon principle (statement and demonstration using potential energy vs. internuclear distance plot), electronic transitions (HOMO, LUMO, bonding, antibonding and non-bonding orbitals, energy level diagram, examples for $\sigma \rightarrow \sigma^*$, $\pi \rightarrow \pi^*$, $n \rightarrow \sigma^*$ and $n \rightarrow \pi^*$ transitions).

λ_{\max} , Chromophores and auxochromes. Bathochromic and hypsochromic shifts. Beer-Lambert's law. Woodward – Fieser rules for calculating λ_{\max} of conjugated dienes and α,β -unsaturated carbonyl compounds. Influence of extended conjugation on the λ_{\max} absorptivity in UV-visible region. Comparison of UV spectra of acetone and methyl vinyl ketone. Effect of conjugation: spectra of 1,3-butadiene, 1,3,5-hexatriene and lycopene.

Applications of Infra-red Spectroscopy

4 Hours

Factors affecting the position of IR absorption peak (atomic and force constant-electronic effects and hydrogen bonding). Regions of IR in the electromagnetic spectrum- (functional group region and finger print regions). Explanation of stretching frequencies of -OH (free and H-bonded), alkyl C-H, alkenyl C-H, and alkynyl C-H stretch frequencies. Group frequencies of N-H, C-C, C=C, C-O and C=O functionalities. IR spectra of benzene, ethanol, phenol, acetaldehyde, acetone and acetic acid and their individual identification.

Nuclear Magnetic Resonance Spectroscopy

6 Hours

Basic principles of proton magnetic resonance: Nuclear magnetic spin quantum number I, the influence of the magnetic field on the spin of nuclei, spin population, saturation using radio frequency. Nuclear magnetic resonance. Chemical shift (δ values). Internal standard - uses of TMS as reference. Nuclear shielding and de-shielding effects. Equivalent and non-equivalent protons. Effect of: (i) electronegativity of adjacent atoms (ii) magnetic induction by pi (π -) electrons- Magnetic anisotropy on chemical shift values. Spin-spin splitting and spin-spin coupling. ¹H NMR spectra of simple organic compounds. Combined Spectral Problems.

References and Recommended Books

1. Physical Chemistry, P. W. Atkins, Julio dePaula, ELBS, 7th edition, (2002).
2. Physical Chemistry: A Molecular Approach, McQuarrie and Simon, Viva, New Delhi, (2001).
3. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).

4. Quantum Chemistry, Ira. N. Levine, PrenBce Hall, New Jersey, (1991).
5. Quantum Chemistry, R. K. Prasad, New Age International, 2nd edition, (2000).
6. Quantum Chemistry through problems and solutions, R. K. Prasad, New Age International (1997).
7. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).
8. Principles of Chemical Kinetics - House J. E. Wm C Brown Publisher, Boston, (1997).
9. Kinetics and Mechanism - A. A. Frost and R. G. Pearson, John-Wiley, New York, (1961).
10. Chemical Kinetic Methods - C. Kalidas, New Age International Publisher, New Delhi (1995)
11. Biochemistry, - Geoffrey Zubay, 2nd Edn., Macmillan Publishing Co. New York (1981).
12. Kinetics and Mechanism of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan..
13. Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata Mc- Graw-Hill: New Delhi (2006).
14. Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.
15. Kemp, W. Organic Spectroscopy, Palgrave
16. Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
17. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

Chemistry VI Practical: Advanced Physical Chemistry and Spectroscopy Practical I

CREDITS: 2

NO. OF HOURS PER WEEK:4

Course Code: 21VCHP6P

Course Objectives:

This course aims to impart to the student skills and knowledge required for

- Preparation and standardization of solutions required for an experiment.
- Use of a colorimeter in the study of the kinetics of a reaction.
- Use of a colorimeter for titrations.
- Use of a colorimeter in the estimation of mixtures.
- Determination of partial molal volume of solutions
- The use of a conductivity meter for determination of specific conductance and solubility of electrolytes
- The use of conductivity meter for titrations (acid base, redox, precipitation).
- Plotting of data in two dimensions and identifying the end point of the titration.
- The working, calibration and use of a potentiometer.
- The use of different reference and working electrodes.
- Methodology of a potentiometric titration for different classes of reactions: acid base, redox, precipitation.

Course Specific Outcomes:

On completion of the course, students should be able to:

- Identify wavelength of maximum absorbance
- Collect data using a colorimeter/spectrophotometer.
- Use colorimeter/spectrophotometer for colorimetric estimations, titrations and kinetic studies.
- Calculate the molal volume of a system at STP using experimental data.
- Learn to work in teams and present experimental results in both oral and written form.
- Use the conductivity meter as a tool for quantitative analysis
- Use conductivity measurements to distinguish between electrolytes (strong and weak)
- Identify problems where conductivity measurements can be used and devise protocols for the experiment.
- Carry out an experiment based on the protocol and find solutions to problems encountered during the experiment
- Use the potentiometer as a tool for quantitative analysis
- Identify problems where potentiometry measurements can be used and devise protocols for the experiment.
- Carry out the experiment based on the protocol and solve problems encountered during the experiment.

Part A

1. Verification of Beer's Law for Cu^{2+} ions
2. Verification of Beer's Law for Fe^{2+} ions
3. Estimation of Fe^{2+} ions concentration in the given solution by titration of FAS versus KMnO_4 through colourimetric method.
4. Estimation of Fe^{2+} ions concentration using EDTA through colourimetric method
5. Phase diagram of two-component systems and determination of E_c , E_T and the determination of the composition of given unknown.
6. Determination of the partial molar volume of solute - H_2O system by apparent molar volume method.
7. Determination of the viscosity of a mixture by apparent molar volume method.

Part B

1. Precipitation titration: conductometric titration of lithium sulphate versus BaCl_2
2. Conductometric titration of weak acid versus weak base.
3. Determination of single electrode potential of Cu^{2+}/Cu and estimate the given unknown concentration.
4. Determination of single electrode potential of Zn^{2+}/Zn and estimate the given unknown concentration.
5. Potentiometric titration of AgNO_3 versus KCl
6. Titration of weak acid against a strong base using quinhydrone electrode and calculation of pK_a and K_a values of the weak acid.
7. Determination of pH of a buffer by using a quinhydrone electrode and comparison of the pH values obtained with glass electrode.

References and Recommended Books

1. Findlay's practical physical chemistry revised by P. B. Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966)
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988)
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987)
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968).
7. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962)
8. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983)
9. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age

International, New York (2001)

10. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co. New York. Delhi (2006).



JYOTI NIVAS COLLEGE AUTONOMOUS, BANGALORE- 560095

III B.Sc., V Semester, 21VCH6T

Chemistry VI

Advanced Physical Chemistry and Spectroscopy I

End Semester Question Paper Format for Theory

Maximum Marks: **60**

Time: **2 Hrs 30 mins**

The question paper shall have **Sections A, B and C**. **Section A** shall consist of **9** questions of **2** marks each of which the student answers **5** questions. **Section B** shall consist of **8** questions of **4** marks each of which the student answers **5** questions. **Section C** shall consist of **4** questions of **10 (can be split as 5+5 and 6+4)** marks of which the student answers **3** questions to give due weightage to all chapters. The question paper shall consist of questions drawn from the respective chapters such that the marks allotted to these chapters are in proportion to the number of teaching hours prescribed. **Paper setters are requested to avoid 2 marks questions in Section B.**

Blue print of Question Paper

Unit	Chapter Title	Hours of Teaching	Marks Allotted
I	Chemical Kinetics	15	23
	Photochemistry	(10+5)	(15+8)
II	Electrochemistry II	15	22
	Quantum Mechanics II	(9+6)	(14+8)
III	Introduction to Spectroscopy	15 (1+4+8+2)	23
	Rotational Spectroscopy		(2+6+12+3)
	Vibrational Spectroscopy		
	Raman Spectroscopy		
IV	Electronic Spectroscopy	15 (5+4+6)	22
	Application of Infra-Red Spectroscopy		(8+6+8)
	Nuclear Magnetic Resonance Spectroscopy		
Total		60	Sec A: 9 x 2 = 18 Sec B: 8 x 4 = 32 Sec C: 4 x 10 = 40 Total = 90
Max. Marks for students: 60 (A: 5 x 2=10 + B: 5 x 4 = 20 + C: 3 x 10 = 30)			



JYOTI NIVAS COLLEGE AUTONOMOUS, BANGALORE- 560095

III B.Sc., V Semester, 21VCH6T

Chemistry VI

Advanced Physical Chemistry and Spectroscopy I

Model Question Paper

Time: 2 Hours 30 Minutes

Max. Marks: 60

Section A

Answer any five of the following questions.

(5 x 2 = 10)

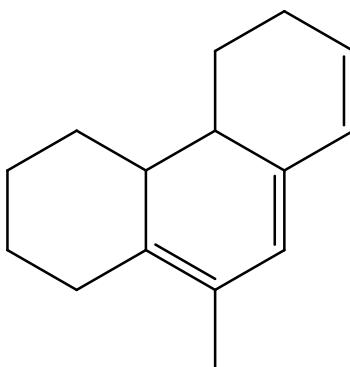
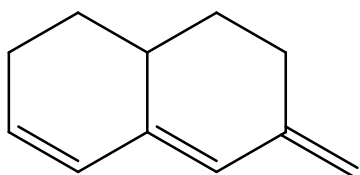
1. Give the significance of energy of activation.
2. What is Photosensitized reaction? Give an example.
3. Why does zinc displace copper from solution and not the other way around?
4. What is an eigenvalue equation? is $\sin x$ an eigenfunction of d/dx ?
5. State the Born-Oppenheimer approximation.
6. What is a group frequency? What is the characteristic peak exhibited by carbonyl compounds?
7. The spectrum of propanone shows a strong UV absorption at 198 nm and a smaller band at 245 nm. Assign transitions to these peaks.
8. What are the different regions of the IR spectrum?
9. Give the expression for the frequency of nuclear spin transition and explain the terms.

Section B

Answer any five of the following questions.

(5 x 4 = 20)

10. The rate constant of a second order reaction is $5.7 \times 10^{-5} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 25° and $1.64 \times 10^{-4} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 40°C . Calculate the activation energy and Arrhenius pre-exponential factor.
11. Explain fluorescence and phosphorescence using Jablonski diagram.
12. Explain how the SHE and calomel electrodes work and how they are constructed.
13. Explain the application of the Shrodinger equation to a particle in a 3D box.
14. The rotation spectrum of $^{12}\text{C}^{16}\text{O}$ has equally spaced lines with a distance of 3.84235 cm^{-1} . If the absolute mass of hydrogen is $1.673 \times 10^{-27} \text{ kg}$, calculate the bond length of carbon monoxide in angstrom units.
15. Sketch the vibrational modes of CO_2 along with the polarisability ellipsoid and explain which modes are Raman active.
16. Calculate the λ_{max} for the following conjugated dienes.



17. What is the compensation method of measuring the EMF of the cell?

Section C

Answer any three of the following questions.

(3 x 10 = 30)

18. (a) Derive an expression for rate constant based on Collision theory.

(b) What is called chain reaction? Explain each stage of chain reaction. (5+5)

19. (a) Derive the Nernst equation.

(b) Explain the pH determination using glass and quinhydrone electrodes. (5+5)

20. (a) Derive expressions for the fundamental, first and second overtone in IR spectroscopy.

(b) Explain the rotation vibration spectra of linear molecules. (5+5)

21. (a) Using the Franck-Condon principle, explain the intensities of vibronic transitions.

(b) Explain the IR spectrum of acetone and acetic acid. (5+5)
