Paper-1 (Theory)

Course Title: Quantum Mechanics and Analytical Techniques

Programme: Diploma in Chemical Dynamics and Analytical Techniques	Year: Two	SEMESTER-IV
Subject: **Chemistry**		
Course Code: BO20401T	**Course Title:** Quantum Mechanics and Analytical Techniques	

Course Outcomes:: Upon successful completion of this course students should be able to describe atomic structure, elementary quantum mechanics ,wave function and its significance ;Schrodinger wave equation and its applications; Molecular orbital theory, basic ideas – Criteria for forming molecular orbital from atomic orbitals , Molecular Spectroscopy, Rotational Spectrum ,vibrational Electronic Spectrum: photo chemistry and kinetics of photo chemical reaction

Analytical chemistry plays an enormous role in our society, such as in drug manufacturing, process control in industry, environmental monitoring, medical diagnostics, food production, and forensic surveys. It is also of great importance in different research areas. Analytical chemistry is a science that is directed towards creating new knowledge so that chemical analysis can be improved to respond to increasing or new demands.

- Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
- Students will be able to function as a member of an interdisciplinary problem solving team.
- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems
- Students will gain an understanding of how to determine the structure of organic molecules using IR and NMR spectroscopic techniques
- To develop basic skills required for purification, solvent extraction, TLC and column chromatography

Credits: 4	Elective
Max. Marks: 25+75	Min. Passing Marks:……

Total No. of Lectures- = 60

Unit	Topics	No. of Lectures
I	**Atomic Structure:** Idea of de-Broglie matter waves, Heisenberg uncertainty principle, atomic orbitals, Schrödinger wave equation, significance of Ψ and Ψ^2, quantum numbers, radial and angular wave functions and probability distribution curves, shapes of s, p, d, orbitals. Aufbau and Pauli exclusion principles, Hund's multiplicity rule.	5
II	**Elementary Quantum Mechanics** : Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids, Bohr's model of hydrogen atom (no derivation) and its defects,	10

	Schrödinger wave equation (time dependent and time independent) and its importance, physical interpretation of the wave function, postulates of quantum mechanics, particle in a one dimensional box. Schrödinger wave equation for H-atom, separation into three equations (without derivation), quantum numbers and their importance, hydrogen like wave functions, radial wave functions, angular wave functions. Molecular orbital theory, basic ideas – Criteria for forming MO from AO, construction of MO by LCAO – H_2^+ ion, calculation of energy levels from wave functions, physical picture of bonding and anti-bonding wave functions, concept of σ, σ*, π, π* orbitals and their characteristics.	
III	**Molecular Spectroscopy**: Introduction: Electromagnetic radiation, regions of the spectrum, basic features of different spectrometers, statement of the Born-Oppenheimer approximation, degrees of freedom **Rotational Spectrum**:Diatomic molecules . Energy levels of a rigid rotor (semi-classical principles), selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of non-rigid rotor, isotope effect . **Vibrational Spectrum:** Infrared spectrum : Energy levels of simple harmonic oscillator, selection rules, pure vibrational spectrum, intensity, determination of force constant and qualitative relation of force constant and bond energies, effect of anharmonic motion and isotope on the spectrum, idea of vibrational frequencies of different functional groups. **Raman spectrum:** Concept of polarizability , pure rotational and pure vibrational, Raman spectra of diatomic molecules, selection rules. Electronic Spectrum: Concept of potential energy curves for bonding and antibonding molecular orbitals, qualitative description of selection rules.	10
IV	**UV-Visible Spectroscopy :** Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules. Types of electronic transitions, λmax, chromophores and auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; application of Woodward Rules for calculation of λmax for the conjugated dienes: alicyclic, homoannular and heteroannular; extended conjugated systems distinction between cis and trans isomers (Cis and trans stilbene) .	5
V	**Infrared Spectroscopy:** **IR Spectroscopy**: Fundamental and non-fundamental molecular vibrations; Hooke's law selection rule, IR absorption positions of various functional groups (C=O, OH, NH, COOH and nitile) , Effect of H-bonding, conjugation, resonance and ring size of cyclic ketones and lactones on IR absorptions; Fingerprint region and its significance; application in functional group analysis and and interpretation of I.R. spectra of simple organic compounds.	5

VI	**^{1}H-NMR Spectroscopy (PMR)** NMR Spectroscopy: introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; choice of solvent and internal standard; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of first-order multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR ; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds; interpretation of NMR spectra of simple compounds. Applications of IR, UV and NMR spectroscopy for identification of simple organic molecules such as Ethanol, Ethyl acetate, acetone, acetaldehyde, dimethylformamide, Cis and trans 1,2-dimethyl cycloprpanone, propene , vinyl chloride, acetophenone, benzaldehyde, phenol, Toluene and ethyl benzene.	10
VII	**Introduction to Mass Spectrometry:** Principle of mass spectrometry, the mass spectrum, mass spectrometry diagram, molecular ion, metastable ion, fragmentation process, McLafferty rearrangement.	3
VIII	**Separation Techniques: Solvent** extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non-aqueous media. Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods.	07

Suggested Readings:

1. Alberty,R A, Physical Chemistry,4 th editionWiley Eastern Ltd ,2001.
2. Atkins,P W,the elements of physical chemistry,Oxford ,1991
3. Barrow,G .M,International student Edition .McGraw Hill, McGraw-Hill,1973.
4. Cotton,F.A, Wilkinson,G and Gaus,P. L ,Basic Inorganic Chemistry,3rd Edition ,Wiley 1995
5. Lee,J.D, Concise Inorganic Chemistry 4th Edition ELBS,1977
6. Clayden, J., Greeves, N., Warren, S., *Organic Chemistry*, Second edition, Oxford University Press 2012.
7. Silverstein, R. M., Bassler, G. C., Morrill, T. C. *Spectrometric Identification of Organic Compounds*, John Wiley and Sons, INC, Fifth edition.
8. Pavia, D. L. *et al*. *Introduction to Spectroscopy*, 5th Ed. Cengage Learning India Ed.
9. Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
10. Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
11. Harris, D.C.: *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.
12. Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.

Suggestive digital platforms web links

1. https://www.coursera.org/courses?query=chemistry&languages=en
2. https://www.mooc-list.com/tags/physical-chemistry
3. https://www.coursera.org/learn/physical-chemistry
4. https://ocw.mit.edu/courses/chemistry/5-61-physical-chemistry-fall-2017/
5. http://heecontent.upsdc.gov.in/Home.aspx
6. https://nptel.ac.in/courses/104/108/104108078/
7. https://nptel.ac.in/courses/104/108/104108124/
8. https://nptel.ac.in/courses/104/106/104106122/

This course can be opted as an elective by the students of following subjects: Chemistry in 12th Class

Suggested Continuous Evaluation Methods: Students can be evaluated on the basis of score obtained in a mid-term exam, together with the performance of other activities which can include short exams, in-class or on-line tests, home assignments, group discussions or oral presentations, among others .

Or

Assessment and presentation of Assignment	(10 marks)
04 Unit tests (Objective): Max marks of each unit test = 10 (average of all 04 unit tests)	(10 marks)
Overall performance throughout the . (Discipline, participation in different activities)	**(**05 marks)

Course prerequisites: To study this course, a student must have had the chemistry in class 12th

Suggested equivalent online courses:
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Further Suggestions:
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Paper-2 (Practical)

Course Title: Instrumental Analysis

Programme: Diploma in Chemical Dynamics and Analytical Techniques	Year: Two	**SEMESTER-IV**
Subject: Chemistry		
Course Code: B020402P	**Course Title: Instrumental Analysis**	

Course outcomes: Upon completion of this course, chemistry majors are able to employ critical thinking and scientific inquiry in the performance, design, interpretation and documentation of laboratory experiments, at a level suitable to succeed at an entry-level position in chemical industry or a chemistry graduate program.

- Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
- Students will be able to function as a member of an interdisciplinary problem solving team.
- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems
- Students will gain an understanding of how to determine the structure of organic molecules using IR and NMR spectroscopic techniques
- To develop basic skills required for purification, solvent extraction, TLC and column chromatography

Credits: 2	Elective
Max. Marks: 25 + 75	Min. Passing Marks:
Practical	**60 h**

Unit	Topics	No of Lectures
I	**Molecular Weight Determination** 1. Determination of molecular weight of a non-volatile solute by Rast method/ Beckmann freezing point method. 2. Determination of the apparent degree of dissociation of an electrolyte (e.g., NaCl) in aqueous solution at different concentrations by ebullioscopy	**10**
II	**Spectrophotometry** 1. To verify Beer – Lambert Law for $KMnO_4/K_2Cr_2O_7$ and determining the concentration of the given solution of the substance from absorption measurement 2. Determination of pKa values of indicator using spectrophotometry. 3. Determination of chemical oxygen demand (COD).	**20**

	4. Determination of Biological oxygen demand (BOD).	
III	**Spectroscopy** 1. Assignment of labelled peaks in the IR spectrum of the same compound explaining the relative frequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C≡C, C≡N stretching frequencies; characteristic bending vibrations are included. Spectra to be provided). 2. Assignment of labelled peaks in the ^{1}H NMR spectra of the known organic compounds explaining the relative δ-values and splitting pattern. 3. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).	**10**
IV	**Chromatographic Separations** 1. Paper chromatographic separation of following metal ions: i. Ni (II) and Co (II) ii. Cu(II) and Cd(II) 2. Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer Chromatography (TLC) 3. Separation and identification of the amino acids present in the given mixture by paper chromatography. Reporting the Rf values 4. TLC separation of a mixture of dyes (fluorescein and methylene blue)	**20**

Suggested Readings:

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.*, Pearson, 2009.
2. Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C.*Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.
5. Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.
6. Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Edition.
7. Mikes, O. & Chalmes, R.A. *Laboratory Handbook of Chromatographic & AlliedMethods*, Elles Harwood Ltd. London.
8. Ditts, R.V. *Analytical Chemistry: Methods of separation.* Van Nostrand, New York, 1974.

Note: For the promotion of Hindi language, course books published in Hindi may be prescribed by the University

Suggestive digital platforms web links

1. https://www.labster.com/chemistry-virtual-labs/
2. https://www.vlab.co.in/broad-area-chemical-sciences
3. **http://chemcollective.org/vlabs**

This course can be opted as an elective by the students of following subjects: Chemistry in 12th Class

Suggested Continuous Evaluation Methods:

Viva voce	(10 marks)
Mock test	(10 marks)
Overall performance	(05marks)

Course prerequisites: To study this course, a student must have had the chemistry in class
Suggested equivalent online courses: ……..
Further Suggestions: ……..