PAPER-VI: QUANTUM CHEMISTRY AND ANALYTICAL TECHNIQUES

Semester	Subject Code	Category	Instruction Hours						Credits
			Lecture		Theory		Practical		
			Per Week	Per Semester	Per Week	Per Semester	Per Week	Per Semester	
II	21CPCH2C	Core	4	60	4	60	0	0	4

COURSE OBJECTIVES

- To learn the principles of quantum mechanics of simple systems, quantum mechanical treatment of multi electron atoms.
- To learn the principles, instrumentation, interpretation and applications of micro wave, IR, Raman spectroscopy, Polarography, Amperometry, Coulometry, various thermal analysis, various elemental analysis and surface analysis techniques

COURSE OUTCOMES:

- On the successful completion of course, students will be able to

CO Number	CO statement	Knowledge level
CO1	Revise and update the mathematical concepts of vectors and tensors to chemical systems by solving eigenvalue and eigenvector problems in matrices and first and second order differential equations that are used for solving the time independent Schrodinger equation, particle in a potential-free box, particle on a ring, harmonic oscillator and particle in a Coulomb potential exactly and demonstrate the solutions for hydrogen atom and molecular rotations and vibrations	**K2 & K3**
CO2	Calculate the energy of simple mujltielectron atoms and molecules, solve all the model problems in quantum mechanics for which exact analytical methods and solutions are available and will apply them to analyze the basis behind the postulatory method of quantum mechanics	**K3 & K2**
CO3	Gain knowledge about the basic principles of rotational and vibrational spectroscopic techniques in different researches	**K3 & K4**
CO4	Acquire knowledge about the basic principles of various electroanalytical techniques such as polarography, amperometry and to study the importance of potentiometric, conductometric and complexometric titration	**K2 & K4**
CO5	Get better understanding of principles, instrumentation and applications of various elemental analysis, surface analysis techniques which will be employed in current research nano projects	**K2 & K3**

* CO-Course Outcomes

Knowledge level K1-Remember; K2-Understand; K3-Apply; K4-Analyze

MAPPING WITH PROGRAM OUTCOMES

COS	PO1	PO2	PO3	PO4	PO5	PO6
CO1	M	M	M	M	S	S
CO2	M	M	S	S	S	M
CO3	M	M	M	M	S	M
CO4	M	S	S	S	S	M
CO5	M	S	S	S	M	S

UNIT-I: QUANTUM CHEMISTRY-I **12 hours**

Black body radiation – Planck's quantum theory – Wave particle duality – Uncertainty Principle. Operators-linear, commutation, Hermitian and Hamiltonian operators – Eigen functions and Eigen values-Postulates of quantum mechanics – Derivation of Schrodinger's time-independent wave equation and its application to particle in a one dimensional box – particle in a three dimensional box, harmonic oscillator, rigid rotor and hydrogen atom.

UNIT-II: QUANTUM CHEMISTRY-II **12 hours**

Born-Oppenheimer approximation-Hydrogen molecule ion – LCAO-MO and VB treatments of the hydrogen molecule – Antisymmetry and Pauli's exclusion principle. Slater detrimental wave function, term symbols and spectroscopic states – Russell Saunders coupling.

Variation theorem – general procedure of variation theorem - Perturbation theory – first order and second order correction. Applications of variation method and perturbation theory to hydrogen and helium atom. Hybridization – determination of bond angles of sp, sp^2 and sp^3 hybridizations – Huckel pi electron (HMO) theory and its applications to ethylene, butadiene and benzene – A brief idea of Hartree and Hartree-Fock self consistent field theory.

UNIT III: ROTATIONAL AND VIBRATIONAL SPECTROSCOPY **12 hours**

Microwave spectroscopy – Theory – selection rules – Instrumentation; Energy levels in atoms and molecules – Fourier transformation Rotational spectra of diatomic and polyatomic molecules – P,Q,R branches – effect of isotopic substitution. Non – rigid rotator – Linear molecules.

Vibrational spectra of diatomic molecules – selection rules – overtones, combination and hot bands - Fermi resonance Energy of diatomic molecule – simple harmonic and unharmonic oscillator, rotational character of vibration spectra.

UNIT-IV: SPECTRO AND ELECTROANALYTICAL TECHNIQUES **12 hours**

X-ray Photoelectron Spectroscopy **(**XPS), Atomic absorption Spectroscopy (AAS), Atomic emission spectroscopy (AES) – Principles, theory, instrumentation and applications – interpretation of spectra – Merits and demerits – Coloumetry – Polarography – theory, apparatus, DME – Diffusion, Kinetic and catalytic currents – Current – voltage curves for reversible and irreversible system – qualitative and quantitative applications to inorganic system.

Amperometric titrations – theory, apparatus, types of titration curves, successive titration and indicator electrodes – Applications. Cyclic voltametry – theory, application to inorganic systems. Potentiometric, conductomertric and complexometric titrations – Masking and demasking agents

UNIT V: SURFACE AND THERMAL ANALYSIS TECHNIQUES 12 hours

Principles, theory, instrumentation and applications of Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray Analysis (EDAX), Atomic Force Microscopy (AFM), Electron Spectroscopy for Chemical Analysis (ESCA) – interpretation of spectra – Merits and demerits.

Principles, theory and applications of Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA), Differential Scanning calorimetry (DSC), Differential Thermogravimetric analysis (DTG). Interpretation of various thermal analysis curves.

Distribution of hours: Theory-70%; Problems-30%

TEXT BOOKS

S.No	Authors	Title	Publishers	Year of publication
1	P. W. Atkins	Molecular Quantum Mechanics	Oxford University Press, Oxford	1983
2	M. W. Hanna, Quantum	Mechanics in Chemistry	W. A Benjamin Inc. London	1965
3	I. N. Levine	Quantum Chemistry	Allyn and Bacon,Boston	1983
4	H. Eyring, J. Walter and G. Kimball,	Quantum Chemistry, Quantum Chemistry	John Wiley and Sons, New York,	1944
5	M. W. Hanna	Mechanics in Quantum Chemistry	W.A. Benjamin Inc. London	1965.
6	G. M. Barrow	Introduction to Molecular Spectroscopy	McGraw Hill, New York	1988.
7	D. A. McQuarrie	Quantum Chemistry	University Science Books, MilValley, California	1998.
8	B. K. Sen.	Quantum Chemistry	Tata McGraw Hill	1992
9	A. K. Chandra	Introduction to Quantum Chemistry	Tata McGraw Hill	1997.
10	W. Levine	Quantum Chemistry	Prentice Hall	1994
11	R. K. Prasad	Quantum Chemistry	Wiley Eastern	1993
12	C. F. Banwell	Fundamentals of Molecular Spectroscopy	McGraw Hill, New York	1966
13	D. A. Skoog and D. M. West	Fundamentals of Analytical Chemistry	Holt Rinehart and Winston Publications, IV Edn	1982
14.	D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch	Fundamentals of Analytical Chemistry	Thomson Asia Pte Ltd., Singapore, 8th Ed	2004

15.	D. A. Skoog	Principles of Instrumental Analysis	Saunders College Pub.Co, 3rd Ed	1985
16.	Willard, Merit, Dean and Settle	Instrumental Methods of Analysis	CBS Publishers and Distributors, 4th Ed	1989
17	G. D. Christian and J. E. O. Reilly	Instrumental Analysis	Allyn and Bacon Inc, 2nd Ed	1986
18	R. S. Drago	Physical methods in chemistry	Reinhold, New York	1968
19	V. K. Ahluwalia	Reduction in Organic Synthesis	CRC Press, 1st Ed	2012

REFERENCE BOOKS

S.No	Authors	Title	Publishers	Year of publication
1.	G.D. Christian and J.E.G. Reily, Allegn	Instrumental Analysis	Becon II Edition	1986
2.	Wilson alld	Comprehensive Analytical Chemistry	Wilson series.	1986
3.	R.C. Kapoor and B.S. Aggarwal	Principles of Polarography	Wiley Easter Limited	1991
4.	Kolthoff and Elwing	Treatise on Analytical Chemistry		
5.	H.A. Strobel, Addison	Chemical Instrumentation	Wesley Publ. Co	1976

TEACHING METHODOLOGY:

- PowerPoint presentation
- Group discussion
- Seminar and Assignments
- Animated videos
- Board and chalk

SYLLABUS DESIGNERS:

1. Dr. T. Gomathi, Assistant Professor, Department of Chemistry
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3. Dr. D. Shakila, Assistant Professor, Department of Chemistry