Semester	**5**
Programme	**CHEMISTRY**
Course	**MAJOR (PHYSICAL CHEMISTRY 4)**
Paper Code	**C3CH230532T/ C3CH230532P**
Credits	**4 (THEORY: 3 1 PRACTICAL: 1)**
Hours/week	**6 (THEORY: 3 1 PRACTICAL: 3)**
Category: Core/MDC/SEC/VEC	**CORE**
Theory/Practical/Composite	**COMPOSITE**
Number of Modules	**3**
Syllabus	**Module –I: Electrochemical Cell (12 Lectures)** 1. Electrical work output: thermodynamic consideration 2. Basic electrostatics 3. Potential difference 4. Electrochemical potential 5. Galvani potential difference at electrode-solution interface 6. Choice of positive and negative electrodes 7. Types of electrodes 8. Coupling of electrodes: electrochemical cell 9. Measuring cell potential 10. Reversible, irreversible cells 11. Electrochemical cells 12. Electrodes 13. Constructing electrochemical cell: liquid-liquid junction and salt bridge 14. Nernst equation for electrode potential: significance 15. Cell potential: its significance 16. Thermodynamics of Galvanic cell 17. Solubility product of a sparingly soluble salt 18. Tabulating standard electrode potential: SHE scale 19. Reference electrode 20. Potentiometric determination of pH of a solution: quinhydrone and glass electrode 21. Concentration cell: electrode and electrolyte concentration cell 22. Electrolyte concentration cell with transference

Module – II Quantum Chemistry (12 Lectures)

1. Diatomic Molecules
2. Separation of electronic and nuclear motion
3. LCAO-MO treatment of H_2^+
4. Bonding and Anti-bonding orbitals
5. Extension to H_2
6. Comparison of LCAO-MO and VB treatments of H_2 and their limitations
7. Dissociation energy
8. Two-centre integrals
9. Valency
10. Approximations in Quantum Chemistry
11. Born-Oppenheimer (B.O.) approximation

Module – III: Liquid state (12 Lectures)

1. Intermolecular forces in liquid.
2. reactivity of a surface molecule.
3. Vapour pressure of a liquid: boiling point.
4. Variation in vapour pressure of a liquid with pressure.
5. Surface tension: force per unit length and energy per unit area interpretation.
6. Liquid drop on a solid surface: contact angle.
7. Variation of shape of the drop: interplay of surface tension between different phases.
8. Shape of liquid meniscus in a capillary.
9. Adhesive and cohesive forces in determining the liquid meniscus in a capillary.
10. Surface energy.
11. Excess pressure: Young and Laplace equation.
12. Capillarity phenomenon.
13. Spreading of liquids: spreading coefficient and Dupre equation.
14. Temperature dependence of surface tension.
15. Measurement of surface tension.

Practicals:

	Introduction to Computer Programming and Numerical Methods Introduction to Fortran 77/ Fortran 90 / C Programming User Defined Functions Subroutines Numerical Methods and their Application in Chemistry a) Root finding of equations. b) Numerical differentiation: difference formula for 1st and 2nd derivative c) Numerical Integration: Trapezoidal rule and Simpson's formula d) Least square method: linear case e) Matrix manipulation: matrix product, Gaussian elimination and the Gauss-Siedel method f) Numerical interpolation g) Extrapolation of data h) Richardson's method Mathematica/Python: Continued Algebraic and numerical calculations using symbolic manipulation programs–Use of Mathematica for simple manipulations.
Course Overview	**Theory:** 1. Description of the thermodynamic properties of reactions that take place in electrochemical cells in which, progress of the reaction drives electrons through an external circuit. Thermodynamic arguments can be used to derive an expression for the electrical potential of such cells and the potential can be related to their composition. The definition of standard potentials is important in this context, in order to predict the equilibrium constants. 2. Quantum mechanical application for the theories of bonding considered for diatomic molecules are introduced as is the variational principle. 3. Study of surfaces is a very important aspect of any comprehensive understanding of chemical reaction dynamics. In solids, the extent to which a surface is covered and variation of the extent of coverage with pressure and temperature is an aspect to be investigated. In liquids, presence of a surface tension requires as rather involved approach from the thermodynamic point of view. **Practical:** Various numerical methods are introduced and applied to solve problems encountered in physical chemistry.

Course Outcomes	Upon successful completion of this course, students will be able to: **CO1:** Apply thermodynamic principles to construct electrochemical cells, calculate electrical work output, and determine standard potentials and the solubility product of sparingly soluble salts. **CO2:** Evaluate irreversible and reversible systems, and utilize potentiometric methods (quinhydrone and glass electrodes) to calculate pH and analyze electrode and electrolyte concentration cells, with and without transference. **CO3:** Implement the Born-Oppenheimer approximation to separate electronic and nuclear motions in diatomic molecules, understanding its theoretical boundaries. **CO4:** Evaluate the bonding and anti-bonding characteristics of diatomic molecules by computing two-centre integrals and dissociation energies, and by comparing the LCAO-MO and Valence Bond treatments for H_2^+ and H_2 systems. **CO5:** Analyze intermolecular forces in the liquid state to explain vapor pressure variations, boiling points, and the energy per unit area interpretation of surface tension. **CO6:** Apply the Young-Laplace and Dupre equations to evaluate capillarity phenomena, the shape of liquid meniscuses, and the spreading coefficients of liquids on solid surfaces, and analyze the temperature dependence and experimental measurement of surface tension. **CO7:** Implement iterative root-finding methods, difference formulas, and Trapezoidal/Simpson's rules to solve algebraic equations and perform numerical integration and differentiation. **CO8:** Execute user-defined subroutines and computational algorithms in Fortran/C/Python to perform matrix manipulations (Gaussian elimination, Gauss-Seidel iteration), least-square linear fitting, numerical interpolation, and data extrapolation (Richardson's method) for chemical analysis, and perform symbolic algebraic computations using Mathematica/Python.

Program Outcomes	**PO1: Fundamental Knowledge:** Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2: Laboratory Skills:** Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3: Problem Solving:** Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. **PO4: Research Competency:** Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5: Interdisciplinary Applications:** Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6: Communication Skills:** Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7: Ethics and Sustainability:** Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	**Course Outcome Statement**	**Bloom's Taxonomy**	**Mapped POs**
CO1	Electrochemical Thermodynamics	**K3 (Apply)**	PO1, PO3
CO2	Cell Potentials & pH Determination	**K4 (Analyze)**	PO1, PO3
CO3	Born-Oppenheimer Approximation	**K3 (Apply), K4 (Analyze)**	PO1, PO3
CO4	Quantum Models of Diatomics (LCAO-MO/VB)	**K5 (Evaluate)**	PO1, PO3
CO5	Liquid State & Surface Tension	**K4 (Analyze)**	PO1, PO3
CO6	Capillarity & Young-Laplace Models	**K3 (Apply), K4 (Analyze)**	PO1, PO3, PO5

CO7	Numerical Integration & Root Finding	**K3 (Apply)**	PO2, PO3
CO8	Computational Algorithms & Matrix Math	**K6 (Create)**	PO2, PO4

Reading/Reference Lists

Theory:

1. Atkins, P. W. & Paula, J. de Atkins', Physical Chemistry, Oxford University Press.
2. Castellan, G. W. Physical Chemistry, Narosa.
3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva.
4. Levine, I. N. Physical Chemistry, Tata McGraw-Hill.
5. Rakshit, P.C., Physical Chemistry, Sarat Book House.
6. Moore, W. J. Physical Chemistry, Orient Longman.
7. Mortimer, R. G. Physical Chemistry, Elsevier.
8. Engel, T. & Reid, P. Physical Chemistry, Pearson.
9. Ball, D. W. Physical Chemistry, Thomson Press.
10. Vemulapalli, G. K, Physical Chemistry, Prentice Hall India.
11. Glasstone, S, Thermodynamics for Chemists, EWP.

Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata McGraw-Hill.

12. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press.
13. Nag, A. K, Physical Chemistry Vol. 1, 2, McGraw Hill.
14. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods Wiley.
15. Sears, F. W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison- Wesley Principles of Physics Series), Pearson; 3rd edition.
16. Metiu, H., Physical Chemistry: Thermodynamics, Taylor and Francis.
17. Kaufman, M., Principles of Thermodynamics, Taylor and Francis.
18. Honig, J. M., Thermodynamics, Academic Press.
19. Levine, I. N. Quantum Chemistry, PHI.
20. Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford.

	21. Eisberg, R., Resnick, R, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 2ed, Wiley. 22. Griffiths, D. J., Introduction to Quantum Mechanics, Cambridge India. 23. Adamson, A. W., Gast, A. P., Physical Chemistry of Surfaces, Wiley. 24. Hiemenz, P. C., Rajagopalan, R., Principles of Colloid and Surface Chemistry, Marcel Dekker. **Practicals:** 1. Mathematics for Physical Chemistry: by D. A. McQuarrie University Science Books 2. Mathematics for Physical Chemistry: by R. Mortimer, Elsevier 3. Chemical Calculations: by P. Yates, CRC Press 4. Physical Chemistry on a Microcomputer: by J. H Noggle, Little Brown & Co. 5. Numerical Recipes in Fortran 77: by W. F. Vetterling, G. A.Teukolsky,B. P. Flannery and W. H. Press, CUP 6. Hildebrand, F. B., Introduction to Numerical Analysis: Second Edition (Dover Books on Mathematics), Dover 7. Boas, M. L., Mathematical Methods in the Physical Sciences 3e, Wiley Riley, K. F., Hobson, M. P., Mathematical Methods for Physics and Engineering: A Comprehensive Guide, Cambridge University Press 1. Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015.
Evaluation	Theory: 60 Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3) Semester Exam: 45 — Practical: 40 CA: 38; Attendance:2
Paper Structure for Theory Semester Exam	Answer THREE out of FOUR questions, of 15 marks each.