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| Semester                                                          | <b>5</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Course                                                            | <b>Major</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Paper Code                                                        | C3CH230532T/ C3CH230532P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Paper Title                                                       | Physical Chemistry 4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| No. of Credits                                                    | 3 Theory + 1 Practical                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Theory / Practical / Composite                                    | Composite                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| Minimum No. of preparatory hours per week a student has to devote | 10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Number of Modules                                                 | 03                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Syllabus                                                          | <p><b>Module –I: Electrochemical Cell (12 Lectures)</b></p> <ol style="list-style-type: none"> <li>1. Electrical work output: thermodynamic consideration</li> <li>2. Basic electrostatics</li> <li>3. Potential difference</li> <li>4. Electrochemical potential</li> <li>5. Galvani potential difference at electrode-solution interface</li> <li>6. Choice of positive and negative electrodes</li> <li>7. Types of electrodes</li> <li>8. Coupling of electrodes: electrochemical cell</li> <li>9. Measuring cell potential</li> <li>10. Reversible, irreversible cells</li> <li>11. Electrochemical cells</li> <li>12. Electrodes</li> <li>13. Constructing electrochemical cell: liquid-liquid junction and salt bridge</li> <li>14. Nernst equation for electrode potential: significance</li> <li>15. Cell potential: its significance</li> <li>16. Thermodynamics of Galvanic cell</li> <li>17. Solubility product of a sparingly soluble salt</li> <li>18. Tabulating standard electrode potential: SHE scale</li> <li>19. Reference electrode</li> <li>20. Potentiometric determination of pH of a solution: quinhydrone and glass electrode</li> <li>21. Concentration cell: electrode and electrolyte concentration cell</li> <li>22. Electrolyte concentration cell with transference</li> </ol> |

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|  | <p><b>Module – II Quantum Chemistry (12 Lectures)</b></p> <ol style="list-style-type: none"> <li>1. Diatomic Molecules</li> <li>2. Separation of electronic and nuclear motion</li> <li>3. LCAO-MO treatment of <math>H_2^+</math></li> <li>4. Bonding and Anti-bonding orbitals</li> <li>5. Extension to <math>H_2</math></li> <li>6. Comparison of LCAO-MO and VB treatments of <math>H_2</math> and their limitations</li> <li>7. Dissociation energy</li> <li>8. Two-centre integrals</li> <li>9. Valency</li> <li>10. Approximations in Quantum Chemistry</li> <li>11. Born-Oppenheimer (B.O.) approximation</li> </ol> <p><b>Module – III: Liquid state (12 Lectures)</b></p> <ol style="list-style-type: none"> <li>1. Intermolecular forces in liquid.</li> <li>2. reactivity of a surface molecule.</li> <li>3. Vapour pressure of a liquid: boiling point.</li> <li>4. Variation in vapour pressure of a liquid with pressure.</li> <li>5. Surface tension: force per unit length and energy per unit area interpretation.</li> <li>6. Liquid drop on a solid surface: contact angle.</li> <li>7. Variation of shape of the drop: interplay of surface tension between different phases.</li> <li>8. Shape of liquid meniscus in a capillary.</li> <li>9. Adhesive and cohesive forces in determining the liquid meniscus in a capillary.</li> <li>10. Surface energy.</li> <li>11. Excess pressure: Young and Laplace equation.</li> <li>12. Capillarity phenomenon.</li> <li>13. Spreading of liquids: spreading coefficient and Dupre equation.</li> <li>14. Temperature dependence of surface tension.</li> <li>15. Measurement of surface tension.</li> </ol> <p><b>Practicals:</b></p> |
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|                   | <p>Introduction to Computer Programming and Numerical Methods</p> <p>Introduction to Fortran 77/ Fortran 90 / C Programming</p> <p>User Defined Functions</p> <p>Subroutines</p> <p>Numerical Methods and their Application in Chemistry</p> <ul style="list-style-type: none"> <li>a) Root finding of equations.</li> <li>b) Numerical differentiation: difference formula for 1st and 2nd derivative</li> <li>c) Numerical Integration: Trapezoidal rule and Simpson's formula</li> <li>d) Least square method: linear case</li> <li>e) Matrix manipulation: matrix product, Gaussian elimination and the Gauss-Siedel method</li> <li>f) Numerical interpolation</li> <li>g) Extrapolation of data</li> <li>h) Richardson's method</li> </ul> <p>Mathematica/Python: Continued</p> <p>Algebraic and numerical calculations using symbolic manipulation programs–Use of Mathematica for simple manipulations.</p>                                                                                                                                                                                                       |
| Learning Outcomes | <p><b>Theory:</b></p> <ol style="list-style-type: none"> <li>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.<br/>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.</li> <li>2. Quantum mechanical application for the theories of bonding considered for diatomic molecules are introduced as is the variational principle.</li> <li>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.<br/>In liquids, presence of a surface tension requires a rather involved approach from the thermodynamic point of view.</li> </ol> |

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|                         | <p><b>Practical:</b></p> <p>1. Various numerical methods are introduced and applied to solve problems encountered in physical chemistry.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Reading/Reference Lists | <p><b>Theory:</b></p> <ol style="list-style-type: none"> <li>1. Atkins, P. W. &amp; Paula, J. de Atkins', Physical Chemistry, Oxford University Press.</li> <li>2. Castellan, G. W. Physical Chemistry, Narosa.</li> <li>3. McQuarrie, D. A. &amp; Simons, J. D. Physical Chemistry: A Molecular Approach, Viva.</li> <li>4. Levine, I. N. Physical Chemistry, Tata McGraw-Hill.</li> <li>5. Rakshit, P.C., Physical Chemistry, Sarat Book House.</li> <li>6. Moore, W. J. Physical Chemistry, Orient Longman.</li> <li>7. Mortimer, R. G. Physical Chemistry, Elsevier.</li> <li>8. Engel, T. &amp; Reid, P. Physical Chemistry, Pearson.</li> <li>9. Ball, D. W. Physical Chemistry, Thomson Press.</li> <li>10. Vemulapalli, G. K, Physical Chemistry, Prentice Hall India.</li> <li>11. Glasstone, S, Thermodynamics for Chemists, EWP. Zemansky, M. W. &amp; Dittman, R.H. Heat and Thermodynamics, Tata McGraw-Hill.</li> <li>12. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press.</li> <li>13. Nag, A. K, Physical Chemistry Vol. 1, 2, McGraw Hill.</li> <li>14. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods Wiley.</li> <li>15. Sears, F. W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition.</li> <li>16. Metiu, H., Physical Chemistry: Thermodynamics, Taylor and Francis.</li> <li>17. Kaufman, M., Principles of Thermodynamics, Taylor and Francis.</li> <li>18. Honig, J. M., Thermodynamics, Academic Press.</li> <li>19. Levine, I. N. Quantum Chemistry, PHI.</li> <li>20. Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford.</li> </ol> |

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