

**SARDAR PATEL UNIVERSITY  
VALLABH VIDYANAGAR**



**SYLLABUS EFFECTIVE FROM: 2018-19  
M.Sc. CHEMISTRY  
SEMESTER-III**

**PHYSICAL CHEMISTRY**

(Total 650 marks)

Subject Code	Subject Name	Hours per week	Internal Marks	External Marks	Total Marks
PS03CPHC21	Molecular Spectroscopic Methods for Structure Determination	4 hrs	30	70	100
PS03CPHC22	Nuclear and Radiation Chemistry	4 hrs	30	70	100
PS03CPHC23	Selected Topics in Physical Chemistry – I	4 hrs	30	70	100
PS03EPHC21-22	Any One	4 hrs	30	70	100
PS03CPHC24	Practicals : Instrumental methods	8 hrs	30	70	100
PS03CPHC25	<b>OR</b> Project work*				
PS03CPHC26	Practicals : Physico-chemical Exercises	8 hrs	30	70	100
PS03CPHC27	<b>OR</b> Project work*				
PS03CPHC28	Comprehensive Viva	1 hrs	-	50	50
Total Marks					650

\* **Project work** (as optional) in place of practicals; to be offered to some of the students, based on their merit, interest and placement with the teachers (Marks : 200). The project shall have to be carried out under the allotted teacher(s) and a dissertation shall be submitted and will be assessed for internal (60 marks) and external (140 marks), in the usual manner.

<b>Paper Code : PS03CPHC21</b>	<b>Total Credits : 4</b>
<b>Title of Paper : Molecular Spectroscopic Methods for Structure Determination</b>	

<b>Unit</b>	<b>Description in detail</b>	<b>Weightage (%)</b>
<b>I</b>	Interaction of radiation with matter, semi-classical treatment, time-dependent perturbation theory and transition rates. Electric dipole, quadrupole and magnetic dipole transition. Selection rule, Line width and line shapes.  <b>UV-spectroscopy :</b> Theory and principles of electronic transition and UV absorption, chromophores and auxochromes, Woodward-Fieser rules, Effect of conjugation, Characteristic absorptions in organic compounds.	<b>25</b>
<b>II</b>	<b>Infra-red and Raman Spectroscopy :</b> Rotation and vibration of diatomic molecules : frequency, force constant, isotopic substitution and energy, selection rules based on spectroscopy and symmetry. Vibrations of polyatomic molecules, classical and quantum mechanical approach, Local and normal modes of analysis and structure with suitable examples. Application of IR and Raman spectroscopy : Geometrical isomerism, metal carbonyls.	<b>25</b>
<b>III</b>	<b><sup>1</sup>H-Nuclear Magnetic Resonance :</b> Origin of Chemical shift and spin-spin coupling, Fourier Transform technique, Pulse sequence, relaxation processes, Use of integration in the quantitative determination of isomers, Factors affecting chemical shifts (inductive, resonance and anisotropic effect with examples), chemical shift of different types of protons (alkane, alkene, alkyne and allene etc.), different spin systems (AB, AM, AX, AB <sub>2</sub> , AX <sub>2</sub> , A <sub>2</sub> B <sub>2</sub> , A <sub>2</sub> X <sub>2</sub> ,....). Factors affecting coupling constants (dihedral angle, Karplus equation-graph, electronegativity, bond order, hybridization, bond angle with examples). Double resonance, spin-spin decoupling, Nuclear Overhauser effect with examples.	<b>25</b>
<b>IV</b>	<b>Mass spectroscopy :</b> Theory, instrumentation, method of ionization (field ionization, FAB, MALDI, californium plasma), different detectors [magnetic analyser, ion cyclotron analyser, quadrupole mass filter], time of flight (TOF). Importance of HRMS, Rules of fragmentation of different functional groups, factors controlling fragmentation examples such as drugs, ionic liquids etc.	<b>25</b>

**Books :**

- Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, 3<sup>rd</sup> Edition, Thomson Brooks/Cole publisher.
- Physical Chemistry, Ira N. Levine, 4<sup>th</sup> Edition, Tata-McGraw Hill Edition.
- Symmetry and Spectroscopy of Molecules, K. Veera Reddy, New Age International Publishers, 2<sup>nd</sup> Edition.

- Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, 1<sup>st</sup> Indian Edition, Brooks/Cole Cengage Learning, 4<sup>th</sup> Edition.
- Molecular Spectroscopy : Theory and Applications, Raman Patel & Raman Patel, University Press, 1<sup>st</sup> Edition.
- Spectroscopy, B. K. Sharma, GOEL Publishing House, 23<sup>rd</sup> Editions.
- Physical Chemistry Through Problems, S. K. Dogra, S. Dogra, New Age International Ltd. Publishers, 2<sup>nd</sup> Edition.
- Atomic and Molecular Spectroscopy, Mool Chand Gupta, New Age International Publishers.
- Physical Chemistry: A Molecular Approach, Donald A. McQuarrie, John D. Simon, Viva Books, Viva Student Edition, Reprint Edn.
- Atomic and Molecular Spectroscopy: Basic concepts and Applications. Rita Kakkal, Cambridge Publication, 1<sup>st</sup> Edition.
- Molecular Spectroscopy, I. N. Levine, Wiley-Interscience Publication.
- Molecular Spectroscopy, J. D. Graybeal, McGraw Hill.
- Modern Spectroscopy, J. M. Hollas, John Wiley & Sons.
- High Resolution Spectroscopy, J. M. Hollas, Butterworths.
- Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, Tata McGraw Hill publishing.

<b>Paper Code : PS03CPHC22</b>	<b>Total Credits : 4</b>
<b>Title of Paper : Nuclear and Radiation Chemistry</b>	

<b>Unit</b>	<b>Description in detail</b>	<b>Weightage (%)</b>
<b>I</b>	<p><b>Nuclear Reactions</b> : Basics, Bathe's notation, Types of nuclear reactions : Elastic Scattering, Photonuclear reaction, Radiative capture, Special nuclear reactions, Evaporation, Fragmentation, Transfer reactions.</p> <p><b>Nuclear Fission</b> : Nuclear shape distortion following excitation, Relation between fission Energy &amp; Fission barrier, Fission parameter.</p>	<b>25</b>
<b>II</b>	<p><b>Nuclear Fusion</b> : Fusion reactions, Basic requirement for controlled thermo nuclear reaction, Threshold conditions, Lawson's criterion, Magnetic confinement (Pinch effect) and Inertial confinement.</p> <p><b>Q value</b> : Q values &amp; Reaction thresholds, Barrier for charged particles.</p>	<b>25</b>
<b>III</b>	<p><b>Radioanalytical techniques and activation analysis</b> :</p> <p><b>Tracer Techniques</b> : Reaction mechanism, Structure determination, Isotope dilution analysis : (i) Direct Isotope dilution analysis (DIDA), (ii) Inverse Isotope Dilution Analysis (IIDA), and (iii) Sub stoichiometric isotope dilution analysis, Dating by tritium content, Dating by <math>^{14}\text{C}</math>, medical applications, Radiometric titrations.</p> <p><b>Neutron Activation Analysis</b> : Principle, Prompt, <math>\tau</math> Neutron activation analysis.</p>	<b>25</b>
<b>IV</b>	<p><b>Radiation Chemistry</b> : Elements, Interaction of radiation with matter.</p> <p><b>Counting Techniques and Radiation dosimetry</b> : Electron multiplication in a gas, The gas counter (Ionization Counter), The Geiger – Muller Counter : (i) Thin end Window Counter; (ii) Thin liquid counter, Proportional Counter.</p> <p>Radiolysis of water, Applications : Radiation induced color centres in the crystals, Chemical and Biological effects of Radiation.</p>	<b>25</b>

**Books :**

- Essential of Nuclear Chemistry, H. J. Arnikar, Wiley Eastern Limited, New Delhi
- Elements of Nuclear Chemistry, R. Gopalan, Vikas Publishing House Pvt. Ltd.
- Nuclear Chemistry, Bernard G. Harvey, Prentice – Hall, Inc., Englewood Cliffs, N. J.
- Radiochemistry and Nuclear Methods of Analysis, W. D. Ehman and D. E. Vance, John Wiley.
- Source book on Atomic Energy. S. Glasstone, Van nostrand Company.

<b>Paper Code : PS03CPHC23</b>	<b>Total Credits : 4</b>
<b>Title of Paper : Selected Topics in Physical Chemistry – I</b>	

<b>Unit</b>	<b>Description in detail</b>	<b>Weightage (%)</b>
<b>I</b>	<b>Statistical Thermodynamics - I :</b> Introduction, Frequency distribution, Binomial, Poisson and normal distribution, Energy states and energy levels, macro states and microstates, thermodynamics probability, the Bose – Einstein statistics, the Fermi – Dirac statistics, the Maxwell – Boltzmann statistics	<b>25</b>
<b>II</b>	<b>Statistical Thermodynamics – II :</b> The statistical interpretation of entropy, the Bose – Einstein distribution function, The Fermi-Dirac distribution function, the classical distribution, comparison of distribution functions for indistinguishable particles, the Maxwell – Boltzmann distribution function, the partition function, thermodynamics properties of system.	<b>25</b>
<b>III</b>	<b>Electrochemistry – I :</b> Introduction, Electrolysis, Arrhenius theory of ionization, Ostwald's dilution law, Application of electrolysis, Ionic atmosphere its radius, Relaxation time, DHO equation and its validity and limitation Wein effect, DH effect, Industrial applications of Electrochemistry : Batteries and Fuel cells	<b>25</b>
<b>IV</b>	<b>Electrochemistry – II :</b> <b>Kinetics of Electrode reactions :</b> Essentials of electrode reactions, Butler-Volmmer model for electrode kinetics, one step, one electron process through potential energy diagram, standard rate constants and transfer coefficients, equilibrium condition and exchange current, current-over potential equation. Very facile kinetics and reversible behaviour, introduction to microscopic theories of charge transfer, Marcus microscopic model, predictions from Marcus theory, Gerischer model based on distribution of energy states, Tunnelling and extended charge transfer	<b>25</b>

**Books :**

- Molecular Statistics for Students of Chemistry, L. A. Woodward Clarendon Press, Oxford.
- Elements of Statistics for Students of Chemistry, L. K. Nash, Wesley Publishing Co., London.
- Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Francis W. Sears, Gerhard L. Salinger, Narosa Publishing House, New Delhi.
- Industrial Electrochemistry, Derek Pletche, Chapman & Hall, New York.
- Modern Electrochemistry, Vol. 1 & 2., J. M. Bockris and A. K. N. Reddy, Plenum Press, New York.
- Electrochemical Methods, A. J. Bard and L. R. Faulkner, John Wiley & Sons, 2<sup>nd</sup> Edition.
- The Principles of Electrochemistry, Duncan A. MacInnes, Dover Publications Inc., New York.
- Electrolytic Solutions, R. A. Robinson and R. H. Stokes, Butterworths, London.

<b>Paper Code : PS03EPHC21</b>	<b>Total Credits : 4</b>
<b>Title of Paper : Surface Chemistry and Catalysis</b>	

<b>Unit</b>	<b>Description in detail</b>	<b>Weightage (%)</b>
<b>I</b>	<p><b>Adsorption</b> : Adsorption definition, Physical and Chemical adsorption – adsorption isotherms : Evaluations, chemisorption on metals and metal oxides, Thermodynamics of adsorption , Langmuir adsorption isotherm, Langmuir constant and Gibbs energy of adsorption, BET adsorption isotherm, adsorption on heterogeneous surface , The potential theory of Polanyi.</p> <p><b>Surface Forces</b> : Van der Waals Forces and macroscopic solids, Microscopic approach, macroscopic calculation – Lifshitz theory, Surface energy and Hamaker constant, Derjaguin approximation, electrostatic double layer, DLVO theory and application.</p>	<b>25</b>
<b>II</b>	<p><b>Micelles, Dispersed Systems and Application</b> : Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC) and methods of determination, factors affecting the CMC of surfactants, counter ion binding of micelles, thermodynamics of micellization – phase separation and mass action models, solubilisation, emulsions, micro-emulsion : Mechanism of formation and their stability, reverse micelles, Micellar catalysis, Photochemistry in micellar systems.</p>	<b>25</b>
<b>III</b>	<p><b>Catalysis – I :</b>  <b>Fundamentals</b> : Catalysis, Concept of activity, selectivity, poisoning, promotion and deactivation. Types of catalysis : homogeneous, heterogeneous, Heterogeneous catalysis and catalytic kinetics : concepts of Langmuir – Hinshelwood</p> <p><b>Preparation and characterization of Catalysts</b> : General methods for preparation of catalysts : precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation of catalysts : calcinations, reduction. Catalyst Characterization : surface area, pore size distribution, particle size determination etc.</p>	<b>25</b>
<b>IV</b>	<p><b>Catalysis – II :</b>  <b>Nanomaterials and Catalysis:</b> General definition, Nano-chemistry basics, distinction between molecules, nanoparticles and bulk materials. Physico-chemical considerations of nanomaterials, Size-dependent properties.</p> <p><b>Catalysis in Green Chemistry and environmental applications</b> : Purification of exhaust gases from different sources, auto-exhaust catalysts (petrol vehicles, diesel vehicles), VOC removal, Ozone decomposition, photocatalysis in effluent treatment</p> <p><b>Photo-catalysis</b> : Photoprocesses at metals, oxides and semiconductors : concepts and mechanism. Photocatalysis application in organic pollutant degradation present in water and air.</p>	<b>25</b>

**Books :**

- Surface Chemistry of Surfactants and Polymers, Bengt Kronberg, Krister Homberg, Bjorn Lindman, Wiley, 1<sup>st</sup> Edition.
- Colloid and Interface Science, Pallab Ghosh, PHI Learning Private Limited.
- Physics and Chemistry of Interface, Hans-Jurgen Butt, Karlheunz Graf, MiCael Kappl, Wiley VCH, 2<sup>nd</sup> Edition.
- Surfactants and Interfacial Phenomena, Milton J. Rosen, Wiley-Interscience, 3<sup>rd</sup> Edition.
- Micelles : Theoretical and Applied Aspects, Yoshikiyo Moroi, Springer Int. Ed.
- Physical Chemistry of Surface, A. W. Admson, Wiley Interscience Publication, 5<sup>th</sup> Edition.
- Surfactant Science and Technology, Drew Myers, VCH Publishers, 2<sup>nd</sup> Edition.
- Principles of Colloids and Surface Chemistry, P. C. Hiemenz, Marcel and Dekker, New York.

<b>Paper Code : PS03EPHC22</b>		<b>Total Credits : 4</b>
<b>Title of Paper : Advanced Characterization Techniques</b>		
<b>Unit</b>	<b>Description in detail</b>	<b>Weightage (%)</b>
<b>I</b>	Mechanical properties of polymers : Introduction, general considerations, objectives, different types of mechanical behaviour, elastic solids and polymer, state of stress and strain, generalized Hook's law. Behaviour of polymers in rubber like state : finite strain elasticity, generalized definition of strain and stress, strain-stress relationship, use of strain energy function, experimental studies of finite elastic behaviour in rubbers.	<b>25</b>
<b>II</b>	Statistical molecular theories of the rubber like state, thermodynamic considerations, statistical considerations. Linear viscoelastic behaviour : viscoelastic behaviour, mathematical treatment of linear of viscoelastic behaviour, dynamical measurements, the complex modulus and complex compliance, the relationship between the complex moduli and the stress relaxation modulus, the relaxation strength	<b>25</b>
<b>III</b>	<b>Rheology :</b> Introduction, Subject and goals, Continuum mechanics as a foundation rheology, Viscoelasticity : liquids, solids, gels, Rheometry experimental methods, analysis and modelling of rheomechanical responses in static and dynamic modes, Applications of rheology in Polymers, Food and processing industries, paint, high energy materials etc. as case studies.	<b>25</b>
<b>IV</b>	<b>Thermal Analysis :</b> <b>Thermogravimetry (TGA):</b> Definition, types of TGA, instrumentation, information from TGA curve, factor affecting TGA curves (instrumental as well as characteristics of sample factors); Application of thermogravimetry, Calculation of percent decomposition and composition of compounds, limitation and advantages of TGA. <b>Derivative thermogravimetry (DTG)</b> and its advantages. <b>Differential Thermal Analysis (DTA) :</b> Definition, Theoretical basis of DTA, Instrumentation for DTA apparatus, Factors affecting the DTA curve, Application of DTA, Advantages and disadvantages of DTA. <b>Differential Scanning Calorimetry (DSC) :</b> General definition, Nano-chemistry basics, distinction between molecules, nanoparticles and bulk materials. Physico-chemical considerations of nanomaterials, Size-dependent properties. <b>Thermo Mechanical Analysis (TMA), Dynamic Mechanical Analysis (DMA) :</b> Instrumentation and Applications.	<b>25</b>

**Books :**

- Mechanical Properties of Solid Polymers, I. M. Ward, Wiley – Interscience, John-Wiley and Sons Ltd., New York.
- Mechanical Properties of Polymers, L. E. Nielson, Reinhold Publishing Co., Chapman and Hall Ltd., London.
- Physical Chemistry of Polymers, A. Tager, Mir Publishers, Moscow.
- Rheology : Concepts, methods and Applications. Alexander Ya. Malkin and Avraam I. Isayev, Chem Tec Publishing, 3<sup>rd</sup> Edition. 2006.



- Introduction to Polymer Rheology, Montgomery T. Shaw, Wiley Publication, 2012.
- Understanding Viscoelasticity, Phan-Thien, Nhan, 2017. Springer Publication.
- Principles of Instrumental Analysis, D. A. Skoog, E. James Holler and S. R. Crouch, Thomson Brooks, 2<sup>nd</sup> Edition.
- Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, Jr., J. A. Dean, F. A. Settlw Jr., CBS Publishers and Distributors, New Delhi, 7<sup>th</sup> Edition.
- Fundamentals of Analytical Chemistry, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, Brooks/Cole Cengage Learning. 8<sup>th</sup> Edition.
- Instrumental Methods of Chemical Analysis, Gurdeep R. Chatwal, Sham K. Anand,
- Introduction to Instrumental Analysis, Pharma Med. Press., Hyderabad, Indian Reprint.
- Instrumental Methods of Chemical Analysis, B. K. Sharma, Goel Publishing House, 28<sup>th</sup> Edition.

<b>Paper Code : PS03CPHC24</b>	<b>Total Credits : 4</b>
<b>Title of Paper : Practicals - Instrumental methods</b>	

- To carry out the following conductometric titrations at room temperature.
  - Solution of a strong acid (hydrochloric acid) with a solution of strong alkali (sodium hydroxide).
  - Solution of a weak acid (acetic acid) with a solution of strong alkali (sodium hydroxide).
  - Solution of a strong acid (hydrochloric acid) with a solution of weak alkali (ammonium hydroxide).
- To determine the stability constant of co-ordination compound (copper-5-sulfosalicylic acid) by pH-metry.
- To titrate pH metrically a phosphoric acid solution against alkali and calculate the first, second and third neutralization or ionization constants of the acid.
- To study the rate equation for the mutarotation of D-glucose in water.
- To determine zero shear viscosity ( $\eta_0$ ) of a polymer solution at different temperatures.
- Investigate the molecular composition of a ferric-salicylate complex by Job's method.
- To determine the rate constant of the saponification of ethyl acetate at different temperatures and calculate the energy of activation of the reaction.
- To study the variation of refractive index with composition of mixtures of carbon tetrachloride and ethyl acetate.
- To find out the amount of Borax in given solution by titrating it against hydrochloric acid pH metrically.
- To determine the decomposition kinetics of a polymer by TGA using iso-conversional method.

**Books :**

- Experiments in Physical Chemistry, J. M. Wilson, R. J. Newcombe, A. R. Denaro, R. M. W. Rickett, Pergamon Press, Oxford.
- Findlay's Practical Physical Chemistry, B. P. Levitt, Longman Group Limited, 9<sup>th</sup> Edition.
- A Laboratory Manual of Experiments in Physical Chemistry, D. Brennan, C. F. H. Tipper, McGraw-Hill Publishing Company Ltd., London.
- Advanced Physico-Chemical Experiments : A Textbook of Practical Physical Chemistry and Calculations. J. Rose, Sir Isaac Pitman & Sons Ltd., London.
- Experimental Physical Chemistry, R. C. Das, B. Behera, Tata McGraw-Hill Publishing Company Ltd., New Delhi.

<b>Paper Code : PS03CPHC26</b>	<b>Total Credits : 4</b>
<b>Title of Paper : Practicals – Physico-chemical Exercises</b>	

1. To investigate the autocatalysis reaction between Potassium permanganate and Oxalic acid.
2. To determine the distribution coefficient of benzoic acid between benzene and water.
3. To determine the formula of the complex ion formed between the cupric ion and ammonia (cuprammonium ion) by distribution method.
4. To determine the rate constant of the oxidation of Iodide ion by hydrogen peroxide in aqueous solutions.
5. To determine the relative strength of HCl and H<sub>2</sub>SO<sub>4</sub> by studying the hydrolysis of methyl acetate.
6. To study the variation in the solubility of calcium hydroxide in the presence of sodium hydroxide and hence, determine the solubility product of calcium hydroxide at room temperature.
7. To study the phase diagram of the ternary system, HAc, H<sub>2</sub>O and CHCl<sub>3</sub>.
8. To determine the molar volume and partial molal volume of given liquid at 25 °C.
9. Kinetics of the reaction of ferric and iodide ions – use of initial rates.
10. To study oscillations chemical reaction (Briggs-Raucher reactions).

**Books :**

- Experiments in Physical Chemistry, J. M. Wilson, R. J. Newcombe, A. R. Denaro, R. M. W. Rickett, Pergamon Press, Oxford.
- Findlay's Practical Physical Chemistry, B. P. Levitt, Longman Group Limited, 9<sup>th</sup> Edition.
- A Laboratory Manual of Experiments in Physical Chemistry, D. Brennan, C. F. H. Tipper, McGraw-Hill Publishing Company Ltd., London.
- Advanced Physico-Chemical Experiments : A Textbook of Practical Physical Chemistry and Calculations. J. Rose, Sir Isaac Pitman & Sons Ltd., London.
- Experimental Physical Chemistry, R. C. Das, B. Behera, Tata McGraw-Hill Publishing Company Ltd., New Delhi.

**OR**

**PS03CPHC25 and PS03CPHC27 :**

**Project work** (as optional) in place of practicals; to be offered to some of the students, based on their merit, interest and placement with the teachers (Marks : 200). The project shall have to be carried out under the allotted teacher(s) and a dissertation shall be submitted and will be assessed for internal (60 marks) and external (140 marks), in the usual manner.

<b>Paper Code:</b> PS03CPHC28	<b>Total Credit: 1</b>
<b>Title of Paper:</b> Comprehensive Viva	

<b>Description in detail</b>	<b>Weightage (%)</b>
Viva Voce From the Subjects Studied in Semester - III	100%