JAI HIND COLLEGE
BASANTSING INSTITUTE OF SCIENCE
&
J.T.LALVANI COLLEGE OF COMMERCE
(AUTONOMOUS)

"A" Road, Churchgate, Mumbai - 400 020, India.

Affiliated to
University of Mumbai

Program: M.Sc. in Chemistry

Course: Physical Chemistry I

Semester I

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2021-22

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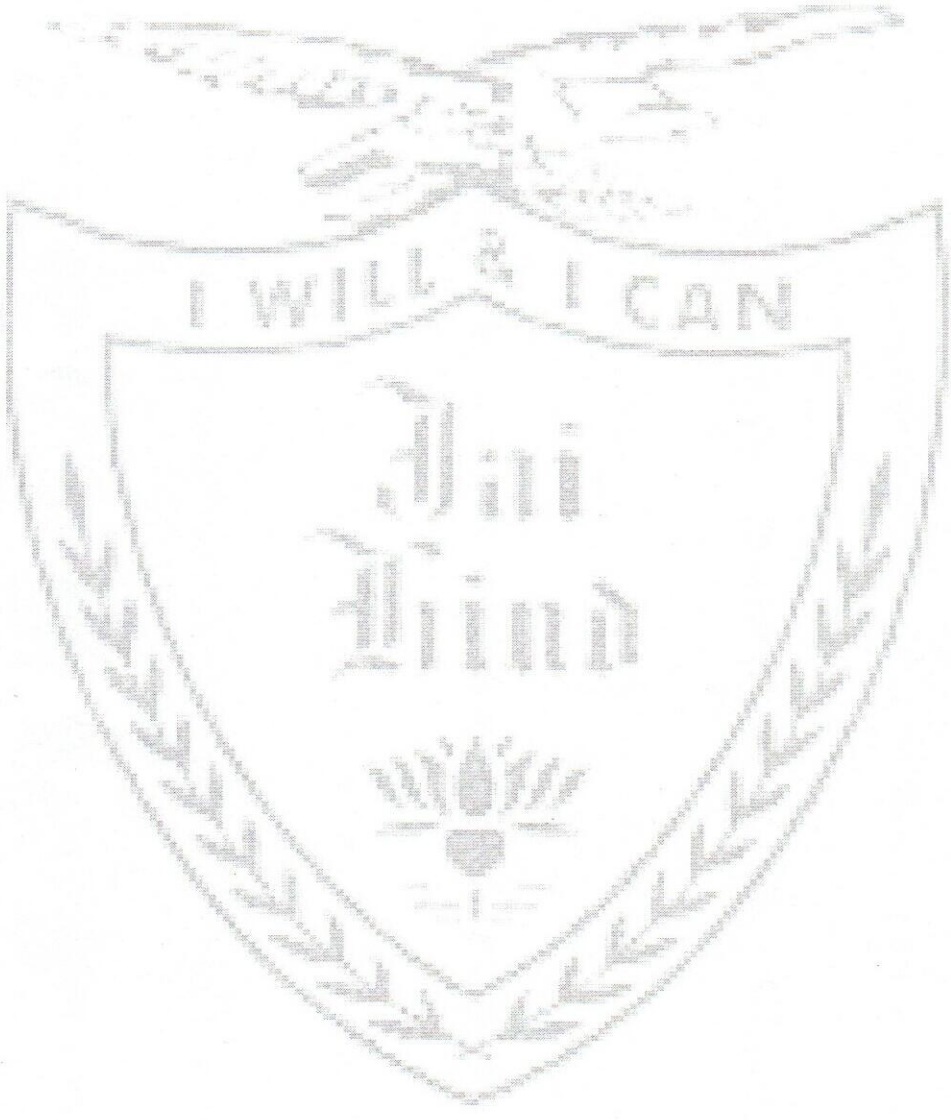
M.Sc. Chemistry Syllabus

Semester I			
Course Code	Course Title	Credits	Lectures/Week
PSCHE101	Physical Chemistry I	04	04



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Semester I

Course Code: PSCHE101	**Course title: Physical Chemistry I**	**Credits: 04 Lectures/Week: 04**
	Course description: Thermodynamics, Quantum Chemistry, Kinetics & Electrochemistry	
	Objectives: **1. To understand the concept thermodynamics.** **2. To Understand the concept of Quantum chemistry and Chemical kinetics.** **3. To recognize the concept of Electrochemistry.** **Outcomes:** **1. To explain concept of thermodynamics, Quantum chemistry, Chemical kinetics and electrochemistry** **2. To solve numerical of thermodynamics, Quantum chemistry, Chemical kinetics and electrochemistry.**	
Unit I	**Chemical Thermodynamics-I** 1.1 State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it's significance and applications to ideal gases, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants. **[8L]** 1.2 Third law of Thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy. **[7L]**	**15L**
Unit II	**Quantum Chemistry-I** 2.1 Quantum theory: failure of classical mechanics, wave particle duality, Heisenberg's uncertainty principle **(2L)** 2.2 Schrodinger's equation for particle waves, wave function & its physical meaning, acceptable wave function, normalization & orthogonality **(4L)** 2.3 Operators & their algebra, linear & Hermitian operators, eigenfunctions & eigenvalues, five basic postulates of quantum mechanics & theorems relating them **(4L)** 2.4 Application of quantum mechanics to the following systems: **(5L)**	**15L**

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	i. Free particles- wave function & energy of a free particle ii. Particle in a box- Particle in a one-, two- and three-dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels. iii. Harmonic oscillator- solution of the equation, energy eigenvalues, physical interpretation of ψ & ψ^2, comparison of classical & quantum mechanical results	
Unit III	**Chemical Dynamics-I** 3.1 Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples Organic Decompositions: Decomposition of ethane, decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits. 3.2 Polymerization reactions: Kinetics of stepwise polymerization, Calculation of degree of polymerization for stepwise reaction. Kinetics of free radical chain polymerization, Kinetic chain length and estimation of average no. of monomer units in the polymer produced by chain polymerization. 3.3 Reaction in Gas Phase Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kasssel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory; Techniques to study gas phase reactions. Fast reactions; relaxation, stop flow and flash photolysis.	**15L**
Unit IV	**Electrochemistry [15L]** 4.1 Recapitulation – basics of electrochemistry. 4.2 Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and its extension to higher concentration (derivations are expected).	**15L**

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	4.3 Electrolytic conductance and ionic interaction, relaxation effect. Debye-Hückel- Onsager equation (derivation expected). Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, Debye -Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect. 4.4 Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells] 4.5 Bio-electrochemistry: Membrane Phenomenon, Bioelectronics [Goldmann equation. (derivations are expected)], Useful preliminaries, Membrane potentials, enzymes as electrodes, electrochemical enzyme-catalysed oxidation of styrene.	

Standard References:

Unit I

1. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7th Edn., Oxford University Press, 2002.
2. *Advanced Physical Chemistry* by Gurtu and Gurtu
3. Puri, B.R.; Sharma, L.R.; Pathania, M.S.; *Principles of Physical Chemistry*, Vishal Publishing Company, 2008.
4. K. L. Kapoor, '*A textbook of Physical Chemistry*' Vol 3, 6th Edition Mc Graw Hill education

Unit II

5. R.K. Prasad, *Quantum Chemistry*, 4th Revised Edn., New Age International Publishers, 2010 (Reprint 2018)
6. Donald A. McQuarrie, *Quantum Chemistry*, 2nd Edition, University Science Books Mill Valley, California
7. Ira R. Levine, *Physical Chemistry*, 5th Edn., Tata McGraw-Hill New Delhi, 2002.

Unit III

8. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7th Edn., Oxford University Press, 2002.
9. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999

Unit IV

10. Bockris, John O'M., Reddy, Amulya K.N., Gamboa-Aldeco, Maria E., *Modern Electrochemistry*, 2A, Plenum Publishers, 1998.
11. *Advanced Physical Chemistry* by Gurtu and Gurtu
12. Puri, B.R.; Sharma, L.R.; Pathania, M.S.; *Principles of Physical Chemistry*, Vishal Publishing Company, 2008.

Additional References:

13. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rd Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
14. McQuarrie, Donald A, and John D. Simon. *Physical Chemistry: A Molecular Approach.*, 1997. Sausalito, Calif.: University Science Books
15. G.W. Castellan, *Physical Chemistry*, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
16. S. Glasstone, *Text Book of Physical Chemistry*, 2nd Edn., McMillan and Co. Ltd.,

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London, 1962
17. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
18. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
19. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
20. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
21. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
22. Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edn., Pearson Education Limited 2013.
23. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st Edn., 1992.

Evaluation Scheme

- **Continuous Assessment (CA) – 40 Marks**
  - Knowledge and Application based: Objective test of 20 Marks
  - Skill based (20 marks): Learner will be assessed on relevant skills pertaining to the course content of a particular paper which could involve but not limited to
    Oral Presentations on relevant topics
    Review writing/Worksheets etc.
- **Semester End Examination (SEE)- 60 Marks**

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Course: Physical Chemistry Practical I

Semester I

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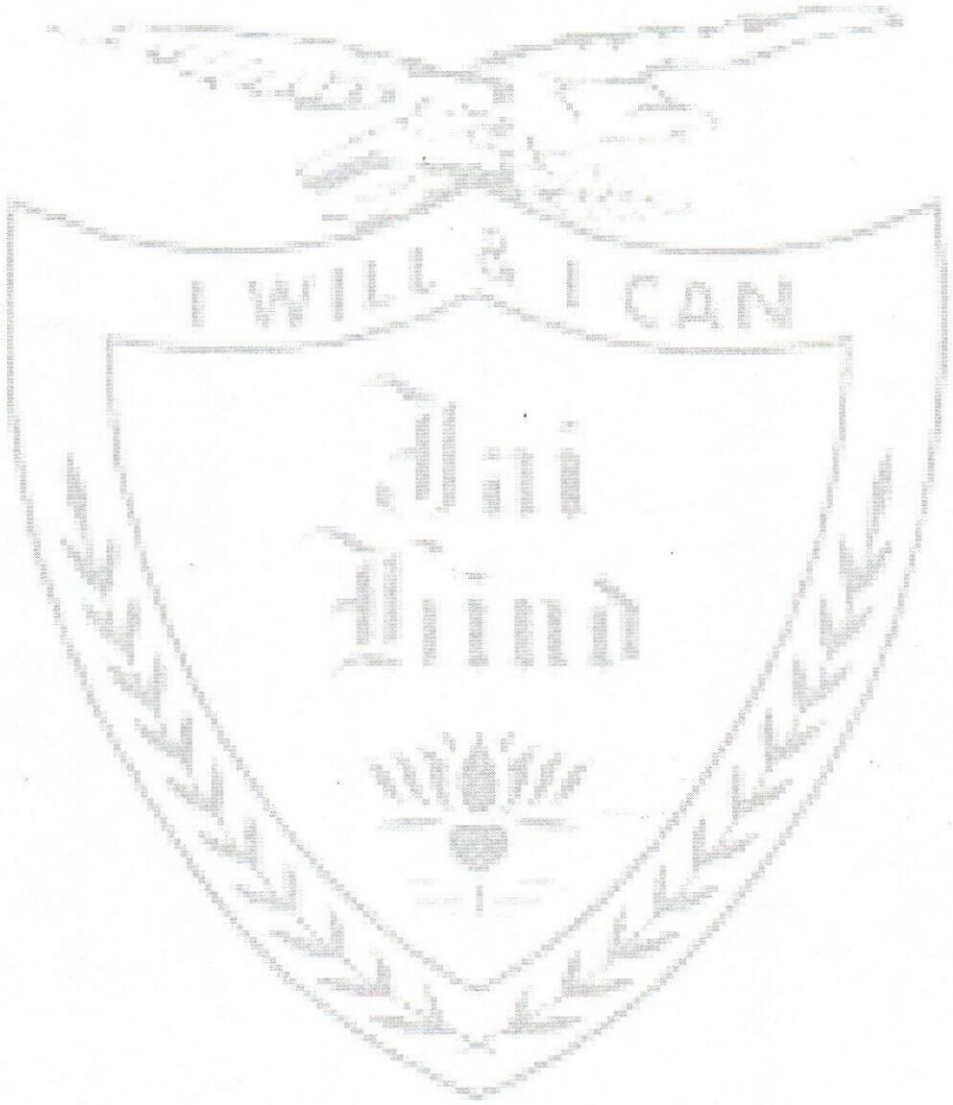
M.Sc. Chemistry Practical Syllabus

Semester I			
Course Code	**Course Title**	**Credits**	**Practical/Week**
PSCHEPR101	**Physical Chemistry Practical I**	**02**	**01**



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Semester I – Practical

Course Code: PSCHEPR101	Course Title: Physical Chemistry Practical I	Credits: 02 Practical/Week

Objectives:

1. **To apply theoretical concepts of thermodynamics, electrochemistry in determination of heat of solutions, solubility products, mean ionic activity and effect of substituents on dissociation constant.**
2. **To understand the concept of Ostwald's dilutions law.**
3. **To explain plotting of graph of mathematical function.**
4. **To discuss the calibration of conductometer and potentiometer instruments.**

Outcomes:

1. **To determine heat of solutions, solubility products, mean ionic activity and effect of substituents on dissociation constant.**
2. **To plot graph of mathematical function.**
3. **To determine dissociation constant of a weak mono-basic acid conductometrically.**

Non-instrumental

1. To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperatures.
2. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of $CaSO_4$ at room temperature.
3. To investigate the reaction between acetone and iodine.
4. To study the variation in the solubility of $Ca(OH)_2$ in presence of NaOH and hence to determine the solubility product of $Ca(OH)_2$ at room temperature.
5. Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?

Instrumental

1. To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2. To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
3. To determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
4. To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.

REFERENCES:

1. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
2. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edn., Longman Group Ltd., 1974.
3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001

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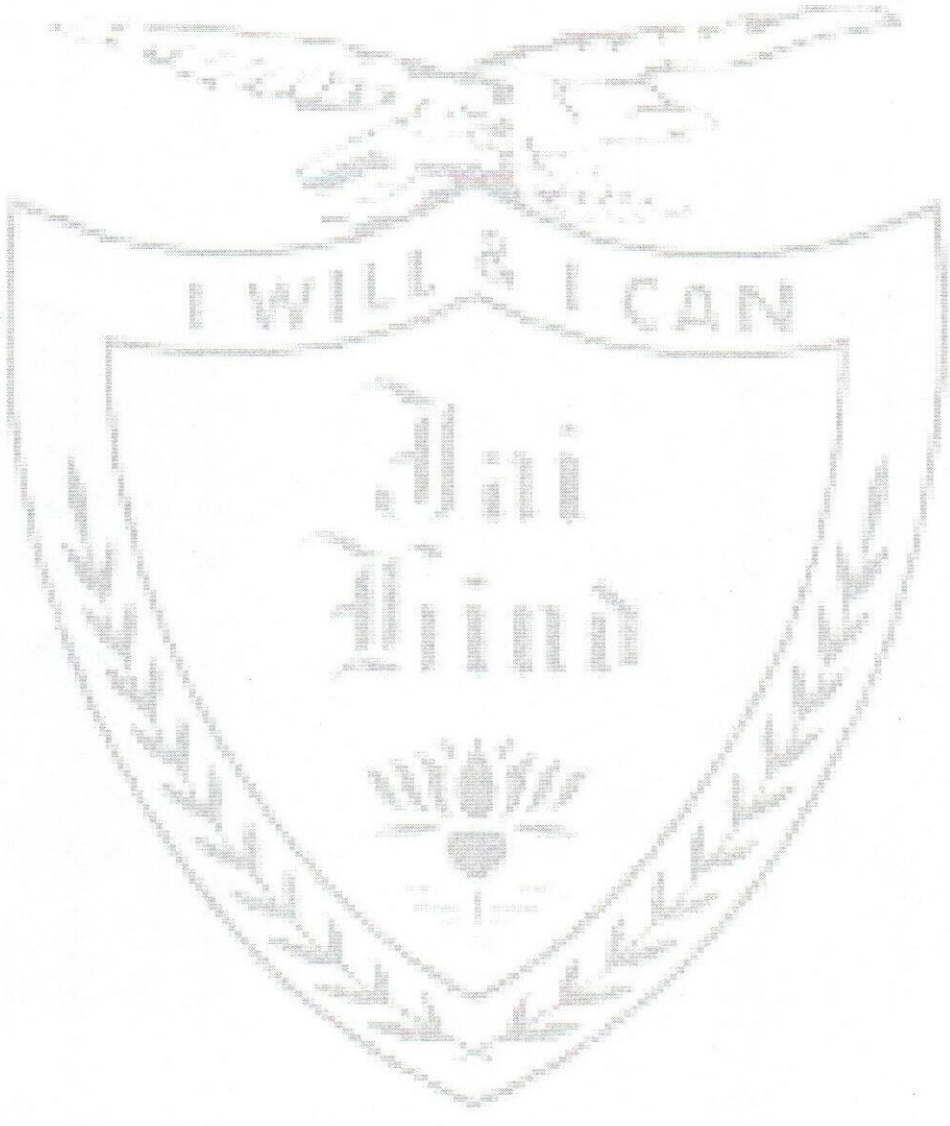
Evaluation Scheme

- **Semester End Examination (SEE)- 50 Marks**



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