# 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
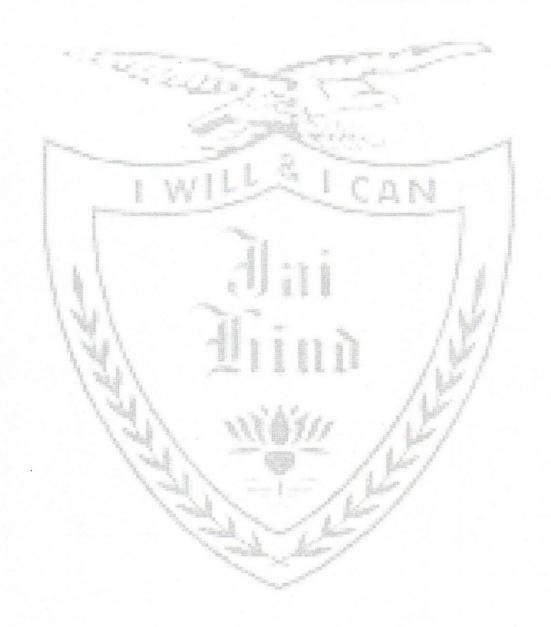
Course: Physical Chemistry II

Semester II

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

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# M.Sc. Chemistry Syllabus

| Semester II | | | |
|---|---|---|---|
| Course Code | Course Title | Credits | Lectures/Week |
| PSCHE201 | **Physical Chemistry II** | 04 | 04 |

| Course Code: PSCHE201 | Course Title: Physical Chemistry II | Credits: 04 Lectures/Week: 04 |
|---|---|---|
| | **Course description:** Thermodynamics, Quantum Chemistry, Kinetics, Solid State Chemistry & Phase Equilibria | |
| | **Objectives:** <br> 1. To understand the advanced concept thermodynamics. <br> 2. To Understand the advanced concept of Quantum chemistry and Chemical kinetics. <br> 3. To recognize the concept of solid state and phase rule. <br> **Outcomes:** <br> 1. To explain concept of thermodynamics, Quantum chemistry, Chemical kinetics and solid state and phase rule. <br> 2. To solve numerical of thermodynamics, Quantum chemistry, Chemical kinetics and solid state and phase rule. | |
| Unit I | **Chemical Thermodynamics-II** <br><br> 1.1 **Fugacity of real gases:** Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing.**[4L]** <br><br> 1.2 **Real Solutions:** Chemical potential in non ideal solutions excess functions of non ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation.**[4L]** <br><br> 1.3 **Thermodynamics of Surfaces:**Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).**[5L]** <br><br> 1.4 **Bioenergetics:**standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.**[2L]** | 15L |
| Unit II | **Quantum Chemistry-II** <br><br> 2.1 **Rigid rotor:** particle in a ring, particle on a sphere, spherical coordinates, Schrödinger wave equation in spherical coordinates, separation of variables, solution of phi and theta equations, spherical harmonics, quantisation of energy. **(4L)** <br><br> 2.2 **Hydrogen atom:**Solution of Schrödinger equation for H-atom, radial eigenfunctions, total wave functions for 1s, 2s, 2p & 3d orbitals, quantum numbers & their significance, atomic orbitals in their real forms. **(4L)** | 15L |

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| | **2.3 Graphical representation of orbitals:** radial & angular plots, radial and angular probability distributions.**(2L)**<br><br>**2.4 Multi-electron systems:** Application of Schrödinger equation for multi-electron system- limitations & introduction to approximation methods.**(1L)**<br><br>**2.5 Hückel Molecular Orbital Theory:** Derivation & application to conjugated systems like ethylene, 1,3-butadiene, benzene.**(4L)** | |
| **Unit III** | **Chemical Kinetics & Molecular Reaction Dynamics**<br><br>**3.1 Elementary Reactions in Solution:** Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action**[4L]**<br><br>**3.2 Kinetics of reactions catalyzed by enzymes:** Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses. **[2L]**<br><br>**3.3 Inhibition of Enzyme action:** Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.**[4L]**<br><br>**3.4 Kinetics of reactions in the Solid State:-** Factors affecting reactions in solids; Rate laws for reactions in solid: The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies.**[5L]** | **15L** |
| **Unit IV** | **SolidState Chemistry & Phase Equilibria**<br><br>**4.1 Solid State Chemistry [6L]**<br><br>   a. Recapitulation: Structures and Defects in solids.<br>   b. Types of Defects and Stoichiometry: Zero dimensional (point), One dimensional (line), Two dimensional (Planar), Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it.<br><br>**4.2 Phase Equilibria [9L]**<br><br>   a. Recapitulation: Introduction and definition of terms involved in phase rule; thermodynamic derivation of Gibbs Phase Rule.<br>   b. Two component system:<br>     i. Solid-Gas system: hydrate formation, amino compound formation | **15L** |

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| | ii. Solid-Liquid system: formation of compounds with congruent and incongruent melting points with suitable examples. |
| | c. Three Component system: |
| |    i. Type I: Formation of one pair of partially miscible liquids |
| |    ii. Type-II: Formation of two pairs of partially miscible liquids |
| |    iii. Type-III: Formation of three pairs of partially miscible liquids |

**Standard References:**

Unit I

1. Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry*, 7th Edn., Oxford University Press, 2002.
2. Puri, B.R.; Sharma, L.R.; Pathania, M.S.; *Principles of Physical Chemistry*, Vishal Publishing Company, 2008.
3. K. L. Kapoor, *'A textbook of Physical Chemistry'* Vol 2, 6th Edition Mc Graw Hill education
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. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
9. Principles of Chemical Kinetics, 2nd Ed., James E. House, ELSEVIER, 2007

Unit IV

10. Solid State Chemistry [An Introduction], 3rd Ed., Lesley E. Smart & Elaine A. Moore, Taylor & Francis, 2010.
11. Principles of the Solid State, H.V. Keer, New Age International Publishers, 2011.
12. Advanced Physical Chemistry by Gurtu and Gurtu
13. Puri, B.R.; Sharma, L.R.; Pathania, M.S.; *Principles of Physical Chemistry*, Vishal Publishing Company, 2008.
14. K. L. Kapoor, *'A textbook of Physical Chemistry'* Vol 3, 6th Edition Mc Graw Hill education

**Additional References:**

15. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7th Edn., Oxford University Press, 2002.
16. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rd Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
17. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
18. McQuarrie, Donald A, and John D. Simon. *Physical Chemistry: A Molecular Approach.*, 1997. Sausalito, Calif.: University Science Books
19. G.W. Castellan, *Physical Chemistry*, 3rd Edn., Narosa Publishing House, New Delhi, 1983.

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20. S. Glasstone, *Text Book of Physical Chemistry*, 2nd Edn., McMillan and Co. Ltd., London, 1962
21. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
22. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
23. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
24. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
25. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
26. Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edn., Pearson Education Limited 2013.
27. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st Edn., 1992.
28. The Physics and 'Chemistry of Solids, Stephen Elliott, Willey India, 2010
29. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 1996.
30. Principles of physical Chemistry , Marrown and Prutton 5th edition
31. Essentials of Physical Chemistry , Arun Bahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
32. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
33. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd ,2011
34. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , CambridgeUniversity Press.

# 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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Program:  M.Sc. in Chemistry

Course: Physical Chemistry Practical II

Semester II

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## M.Sc. Chemistry Practical Syllabus

| Semester II | | | |
| --- | --- | --- | --- |
| Course Code | Course Title | Credits | Practical/Week |
| PSCHEPR201 | **Physical Chemistry Practical II** | 02 | 01 |

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## Semester II – Practical

| Course Code: PSCHEPR201 | Course title: Physical Chemistry Practical II | Credits: 02 Practical/Week: 01 |
|---|---|---|
| | **Objectives:** <br> 1. To inculcate aptitude for experimentation and treatment of data in learners. <br> 2. To recapitulate the theory of the ionic strength, phase rule, chemical kinetics for experimental determinations. <br> 3. To apply static method for determination of empirical formula o Complex. <br> **Outcomes:** <br> 1. To determine polar plots of atomic orbitals of hydrogen atom. <br> 2. To develop knowledge in finding rate constant of decomposition reaction. <br> 3. To draw phase rule diagram for three component system. <br> 4. To estimateCMC of sodium Lauryl Sulphate. | |
| | **Non-instrumental** <br><br> 1. Polar plots of atomic orbitals such as 1s, 2pz and 3dz2 orbitals by using angular part of hydrogen atom wave functions. <br> 2. To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate. <br> 3. To study the phase diagram of three component system water – chloroform /toluene - acetic acid. <br> 4. To determine the rate constant of decomposition reaction of diacetone alcohol by dialtometric method <br><br> **Instrumental** <br><br> 1. To determine the formula of silver ammonia complex by potentiometric method. <br> 2. To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations. <br> 3. To determine Hammette constant of m- and p- amino benzoic acid/nitro benzoic acid by pH measurement. <br> 4. To determine the Michaelis – Menten's constant value (Km) of the enzyme Beta Amylase spectrophotometrically. <br><br> **REFERENCES:** <br> 1. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005. <br> 2. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edn., Longman Group Ltd., 1974. <br> 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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