

UNIVERSITY OF MADRAS
M.Sc. DEGREE PROGRAMME IN CHEMISTRY
 SYLLABUS WITH EFFECT FROM 2023-2024

Title of the Course	PHYSICAL CHEMISTRY-I						
Paper No.	Core V						
Category	Core	Year	I	Credits	4	Course Code	424C2B
		Semester	II				
Instructional hours per week	Lecture	Tutorial	Lab Practice		Total		
	4	1	-		5		
Prerequisites	Basic concepts of physical chemistry						
Objectives of the course	<p>To recall the fundamentals of thermodynamics and the composition of partial molar quantities.</p> <p>To understand the classical and statistical approach of the functions.</p> <p>To compare the significance of Maxwell-Boltzman, Fermi-Dirac and Bose-Einstein.</p> <p>To correlate the theories of reaction rates for the evaluation of thermodynamic parameters.</p> <p>To study the mechanism and kinetics of reactions.</p>						
Course Outline	<p>UNIT-I: Classical Thermodynamics: Partial molar properties-Chemical potential, Gibb's- Duhem equation-binary and ternary systems. Determination of partial molar quantities. Thermodynamics of real gases - Fugacity- determination of fugacity by graphical and equation of state methods-dependence of temperature, pressure and composition. Thermodynamics of ideal and non-ideal binary mixtures, Duhem - Margulus equation applications of ideal and non-ideal mixtures. Activity and activity coefficients-standard states - determination-vapour pressure, EMF and freezing point methods.</p>						
	<p>UNIT-II: Statistical thermodynamics: Introduction of statistical thermodynamics concepts of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics- comparison and applications. Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions-calculation of equilibrium constants. Statistical approach to Thermodynamic properties: pressure, internal energy, entropy, enthalpy, Gibb's function, Helmholtz function residual entropy, equilibrium constants and equipartition principle. Heat capacity of mono and di atomic gases-ortho and para hydrogen. Heat capacity of solids-Einstein and Debye models.</p>						
	<p>UNIT-III: Irreversible Thermodynamics: Theories of conservation of mass and energy entropy production in open systems by heat, matter and current flow, force and flux concepts. Onsager theory-validity and verification- Onsager reciprocal relationships. Electro kinetic and thermo mechanical effects-Application of irreversible thermodynamics to biological systems.</p>						
	<p>UNIT-IV: Kinetics of Reactions: Theories of reactions-effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis-</p>						

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	<p>molecular beams, collision cross sections, effectiveness of collisions, Potential energy surfaces. Transition state theory-evaluation of thermodynamic parameters of activation-applications of ARRT to reactions between atoms and molecules, time and true order-kinetic parameter evaluation. Factors determine the reaction rates in solution - primary salt effect and secondary salt effect, Homogeneous catalysis-acid- base catalysis-mechanism of acid base catalyzed reactions-Bronsted catalysis law, enzyme catalysis-Michelis-Menton catalysis.</p> <p>UNIT-V: Kinetics of complex and fast reactions: Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. Chain reactions-chain length, kinetics of $H_2 - Cl_2$ & $H_2 - Br_2$ reactions (Thermal and Photochemical reactions) - Rice Herzfeld mechanism. Study of fast reactions-relaxation methods-temperature and pressure jump methods electric and magnetic field jump methods -stopped flow flash photolysis methods and pulse radiolysis. Kinetics of polymerization-free radical, cationic, anionic polymerization - Polycondensation.</p>
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	<p>Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)</p>
Skills acquired from this course	<p>Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.</p>
Recommended Text	<ol style="list-style-type: none"> 1. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd edition, S.L.N.Chand and Co., Jalandhar, 1986. 2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A. Benjamin Publishers, California, 1972. 3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995. 4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013. 5. J. Rajaram and J.C. Kuriokose, Kinetics and Mechanisms of chemical transformation, M acmillan India Ltd, Reprint - 2011.
Reference Books	<ol style="list-style-type: none"> 1. D.A. Mcqurrie And J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999. 2. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi, 1990. 3. S.H. Maron and J.B. Lando, Fundamentals of Physical Chemistry, Macmillan Publishers, New York, 1974 4. K.B. Ytsiimiriski, "Kinetic Methods of Analysis", Pergamom Press, 1996. 5. Gurdeep Raj, Phase rule, Goel Publishing House, 2011.
Website and e-learning source	<ol style="list-style-type: none"> 1. https://nptel.ac.in/courses/104/103/104103112/ 2. https://bit.ly/3tL3GdN

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Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To explain the classical and statistical concepts of thermodynamics.

CO2: To compare and correlate the thermodynamic concepts to study the kinetics of chemical reactions.

CO3: To discuss the various thermodynamic and kinetic determination.

CO4: To evaluate the thermodynamic methods for real gases and mixtures.

CO5: To compare the theories of reaction rates and fast reactions.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to Pos	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low