

KU6DSCCHE302: PHYSICAL CHEMISTRY- III

Semester	Course Type	Course Level	Course Code	Credits	Total Hours
VI	DSC	300	KU6DSCCHE302	4	60

Learning Approach (Hours/ Week)		Marks Distribution			Duration of ESE (Hours)
Lecture/ Tutorial	Practical/ Internship	CE	ESE	Total	
4	-	30	70	100	2

Course Description: The course comprises of modules on thermodynamics and spectroscopy. The course will help students to develop good understanding on thermodynamics and spectroscopy.

Course Prerequisite: Basic idea about thermodynamics

Course Outcomes:

CO No.	Expected Outcome	Learning Domains
1	Comprehensive understanding about the various laws of thermodynamics	U
2	Able to explain the energy changes associated with various process around and predict the feasibility of a process or reaction in scientific way	A
3	Understand the concept of entropy	U
4	Comprehensive understanding of various spectroscopic techniques and able to apply in interpreting the spectra of compounds	A

***Remember (R), Understand (U), Apply (A), Analyse (An), Evaluate (E), Create (C)**

Mapping of Course Outcomes to PSOs

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	PSO 7
CO 1	3	3	3	0	3	3	0
CO 2	3	3	3	0	3	3	1
CO 3	3	3	3	1	3	3	0
CO 4	3	3	3	0	3	3	0

Course Contents for Classroom Transaction:

M O D U L E	U N I T	DESCRIPTION	HO URS
		THERMODYNAMICS -I	10
	1	Basic concepts -- study of terms -- system and surroundings -- open, closed and isolated systems, isothermal, Isochoric – adiabatic systems- state and state variables -- macroscopic properties – intensive and extensive properties - reversible and irreversible processes – work, heat and energy – state functions and path functions.	
1	2	First law of thermodynamics- Internal energy and enthalpy --- zeroth law of thermodynamics –concept of temperature. statement of first law of thermodynamics – conservation of energy – expansion work – general expression for work – work done during free expansion, expansion against constant pressure and isothermal reversible expansion.	
	3	Heat capacity of gases at constant volume C_v and constant pressure C_p – relation between C_p and C_v and its derivation – P, V, T relations during adiabatic process -- work done during reversible adiabatic expansion-	

		comparison for isothermal and adiabatic process -- Change in enthalpy at constant pressure -- Joule Thomson effect -- internal pressure -- inversion temperature	
	4	Thermochemistry- – standard enthalpy changes for physical and chemical processes –enthalpy of -neutralization, transition, formation, phase changes, combustion and solution- heats of reaction at constant volume q_v and constant pressure q_p – relation between q_p and q_v Hess's law and its applications –bond energy calculations-variation of enthalpy change of a reaction with temperature – Kirchoff equation.	

	THERMODYNAMICS II		15
	1	Second law of thermodynamics -Limitations of first law – cyclic process – Carnot cycle – efficiency of heat engine – statement of second law of thermodynamics in terms of work and heat- Clausius, Kelvin Planck statement concept of entropy -- physical significance of entropy (microscopic)– variation of entropy of ideal gases with pressure and temperature	
2	2	Second law in terms of entropy – entropy change for phase transitions – criteria for spontaneous changes-for isolated system at constant (T&V), (T&P), (S&V), (S&P)– Gibbs and Helmholtz free energies – condition of spontaneity in terms of free energy – comparison of entropy and free energy – Gibbs- Helmholtz equation – Maxwell relations	
	3	Partial molar properties – concept of free energy – Gibbs Duhem equation – variation of chemical potential with temperature and pressure. Chemical potential of a component in a mixture of ideal gases. -Third law of thermodynamics-absolute entropy-Clausius- Clapeyron equation	
	4	Derivation of important laws from thermodynamics	
3	SPECTROSCOPY-I		13

	1	Introduction: electromagnetic radiation, regions of the spectrum, interaction of electromagnetic radiation with molecules, Born-Oppenheimer approximation.	
	2	Microwave Spectroscopy – Rotation Spectra-Instrumentation- Moment of inertia, Rotational -Quantum numbers, Rotational Constant, Intensities of rotational spectral lines, Rotational –Vibrational Spectrum of diatomic molecules – Selection rules for rotational spectra.	
	3	Infrared Spectroscopy –Theory of infrared spectra-Degree of freedom in poly atomic molecules, Selection rule, Molecular vibration – Stretching and Bending modes, Calculation of stretching-frequencies – fundamental Bands and Overtones, hot bands and Fermi resonance. Factors influencing vibrational frequency – Electronic effects, hydrogen bonding, solvent effect. Applications of IR Spectroscopy.	

	SPECTROSCOPY-II		10
		Raman Spectroscopy –block diagram, quantum theory of Raman scattering- Stokes and antistokes lines-selection rule, rule of mutual exclusion	
4	2	NMR Spectroscopy -- Introduction, Theory of NMR, Phenomena of resonance, Modes of nuclear spin-Relaxation Process, Chemical Shift – Internal standard, δ and τ scale, Shielding Effects, Factors affecting Chemical Shift, Spin-Spin interaction, Interpretations of spectra of ethyl bromide, ethanol, acetaldehyde, acetone, toluene and acetophenone.	
	3	Mass Spectrometry – Basic principles, Fragmentation pathway, Molecular ion peak, base peak, Meta stable ion, General rules for predicting the prominent peaks, Mc Lafferty Rearrangement, mass spectra of simple alkanes, cycloalkanes, saturated alcohols and aliphatic ketones	

	TEACHER SPECIFIC MODULE	12
	Directions: A module on UV spectroscopy or any other relevant topic as per teacher's choice may be taught	
5	UV Spectroscopy – Franck Condon principle-intensity of spectral lines - Absorption laws, Selection Rules – Types, Electronic transitions – Position and Intensity of absorption, Molar extinction coefficient, Chromophore – Auxochrome Concept, Absorption and Intensity Shifts, Types of Absorption Bands, Interpretations of spectra of simple conjugated dienes and enones, Woodward-Fieser Rule, Application to dienes and enones.	

Essential Readings:

1. Elements of Physical chemistry: Puri, Sharma and Pathania, Vishal Publishing Co
2. Physical Chemistry: W.J. Moore, Orient Longmans.
3. Physical Chemistry: N. Kundu & S.K. Jain, S. Chand & Company
4. Physical Chemistry: N. Kundu & S.K. Jain, S. & Company
5. Physical Chemistry: P.W. Atkins, Oxford University Press
6. Electronic absorption spectroscopy and related techniques: D. N. Satyanarayana, Universities
7. Symmetry and spectroscopy of molecules: K. Veera Reddy, New Age. International(P) Ltd
8. Fundamentals of molecular spectroscopy: C. N. Baanwell and E M Mc Cash, Tata McGraw Hill
9. Physical Chemistry – A molecular Approach: Mc Quarrie, J. D. Simon, Viva Books Pvt Ltd.
10. A Textbook of Physical chemistry: K. L. Kapoor, Volume 4, Macmillan India Ltd.
11. Physical Chemistry, I. N. Levine, Tata Mc Graw Hill.
12. Physical Chemistry, K. J. Laidler, John H. Meiser.

Assessment Rubrics:

Evaluation Type		Marks
End Semester Evaluation (ESE)		70
Continuous Evaluation (CCA)		30
Theory (CCA)		30
a)	Test Paper*	12
b)	Assignment	6
c)	Seminar, Viva-Voce	12
Total		100

*Average mark of the best two written tests may be considered for internal mark.