

KU7DSCCHE404: PHYSICAL CHEMISTRY- V

Semester	Course Type	Course Level	Course Code	Credits	Total Hours
VII	DSC	400	KU7DSCCHE404	4	75

Learning Approach (Hours/ Week)		Marks Distribution			Duration of ESE (Hours)
Lecture/ Tutorial	Practical/ Internship	CE	ESE	Total	
3	2	35	65	100	1.5

Course Description: The comprises of modules on advanced thermodynamics, phase equilibrium, statistical thermodynamics, concepts and applications of nanoscience, practicals on phase equilibrium and nano science.

Course Prerequisite: Knowledge about laws of thermodynamics, Phase rule and quantum chemistry.

Course Outcomes:

CO No.	Expected Outcome	Learning Domains
1	Illustrate the concepts of the third law of thermodynamics and thermodynamic irreversibility.	U
2	Analyze phase transitions and phase diagrams of three component systems	An
3	Correlate the principles of quantum and statistical mechanics	A
4	Understand the methods of synthesis of nanomaterials and its characterization techniques	U

5	Acquire skill in advanced physical chemistry experiments and nano synthesis	A
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**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	1	2	1	2	2	2
CO 2	3	2	2	1	1	2	2
CO 3	3	2	2	2	1	2	2
CO 4	3	1	2	1	1	2	2
CO 5	3	1	2	1	1	2	2

Course Contents for Classroom Transaction:

M O D U L E	U N I T	DESCRIPTION	H O U R S
1	THERMODYNAMICS III		11
	1	Third law of thermodynamics- need for third law, Nernst heat theorem, determination of absolute entropies using third law, Residual entropy. entropy changes in chemical reactions. Thermodynamic equations of state.	
	2	Partial molar quantities - chemical potential-variation of chemical potential with T&P- determination of partial molar volume and enthalpy. Thermodynamic functions of ideal gases, real gases, and gas	

		mixtures- Entropy and free energy of mixing. Excess thermodynamic functions.	
	3	Thermodynamics of irreversible processes with simple examples. The general theory of nonequilibrium processes. Entropy production. The phenomenological relations. Principle of microscopic reversibility, Onsager reciprocal relations	
	4	Application to the theory of diffusion, thermo-osmosis, and Thermoelectricity (Seebeck effect, Peltier effect, and Thomson effect).	

	PHASE EQUILIBRIUM		8
2	1	Phase rule -Physical equilibria involving phase transition-criteria for equilibrium between phases	
	2	Three component system- graphical representations-solid liquid equilibria Ternary solution with common ion-Hydrate formation-compound formation	
	3	Liquid-liquid equilibria-one pair of partially miscible liquids-two pairs of partially miscible liquids-three pairs of partially miscible liquids.	

	STATISTICAL THERMODYNAMICS		18
	1	Distinguishable and Indistinguishable particles, phase space, Ensemble, Macrostates, and microstates. Stirlings approximation- Thermodynamic probability -Derivation of Maxwell-Boltzmann distribution law	
	2	Partition function- physical significance- total partition function; Separation of Molecular partition function - Translational, Rotational, vibrational, electronic and nuclear partition function. Rotational temperature- Fundamental vibrational temperature-Thermal de-Broglie wavelength.	
	3	Heat capacity of gases- Classical and quantum theories-Equipartition principle - Heat capacity of Hydrogen – Ortho and Parahydrogen.	

	4	The atomic crystals: Einstein's theory of atomic crystal - Debye's modification of Einstein's model.	
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	CONCEPTS AND APPLICATIONS OF NANO SCIENCE		7
4	1	Nanomaterials – Classification based on dimensions	
	2	Synthesis – Top down and bottom up-chemical precipitation, mechano-chemical method, micro emulsion method, reduction technique, chemical vapour deposition and solgel method, Hydrothermal synthesis (brief study)	
	3	Important methods for the characterization of nanomaterials – Scanning electron microscopy (SEM)-transmission electron microscopy (TEM).	
	4	Synthesis and applications of Quantum dots-Carbon nanotubes and Graphene (brief study)	

	TEACHER SPECIFIC MODULE-PRACTICALS		
	Minimum 3 experiments must be done. Experiment in nano synthesis is open ended		30
5	a) Solid and liquid equilibria: construction of phase diagram of simple eutectics, systems with congruent melting points, and solid solutions. Determination of the composition of unknown mixtures. Analytical and synthetic methods for the determination of solubilities and heat of solution		
	b) Partially miscible liquids: critical solution temperature, the influence of impurities on the miscibility temperature (KCl, NaCl, and /or succinic acid). Determination of the composition of unknown mixtures.		
	c) Completely miscible systems: construction of phase diagram of a two-component liquid system. Zeotropic and azeotropic		

d) Three-component systems: with one pair of partially miscible liquids. Construction of phase diagrams of tie lines. Compositions of homogenous mixtures.	
Synthesize nano particles of metals or metal oxides/sulphides (open ended)	
Suggestion: Sol -gel method- (ZnO, MgO)	

Essential Readings:

1. S.Glasstone-“Thermodynamics for chemists”–Affiliated East West publication.
2. Rastogi and Misra- “An Introduction to chemical thermodynamics-6th edition”– Vikas publishing
3. I.Pregogine- “Introduction of Irreversible to thermodynamics process”- Interscience
4. Phase Equilibria, Phase Diagrams and Phase Transformations: Their Thermodynamic Basis by M. Hillert
5. Phase Diagrams: Materials Science and Technology, Volume III” by P. Villars and L.D. Calvert
6. M.C.Gupta-“Elements of Statistical Thermodynamics-New age international.
7. L.K.Nash- “Elements of Statistical Thermodynamics-Addison Wesley publishing
8. Kistina and Sorfuran-“A course on statistical thermodynamic”-Academic 1971.
9. D.A. McQuarrie-“Statistical thermodynamic”-Harper and Row 1973.
10. Winston Revie and Herbert Uhlig Corrosion and corrosion control:(Wiley Edited by Sheir, Jarman and Burstein Corrosion Control Volume 2
12. Nanoscience and nanotechnology: V. S. Muraleedharan and A. Subramania, Ane Book Pvt Ltd.
13. Nano; The Essentials: T. Pradeep, Mc Graw-Hill education
14. Lewis and Randal-“Thermodynamics”-McGraw-Hill.

Assessment Rubrics:

Evaluation Type		Marks
End Semester Evaluation (ESE)		65 (50T+15P)
Continuous Evaluation (CCA)		35 (25T+10P)
Theory		25
a)	Test Paper*	10
b)	Assignment	5
c)	Viva-Voce	5
d)	Seminar	5
Practical10		
a)	Skill	4
b)	Record	4
c)	Punctuality	2
Total		100

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