Course No.	Course Name	L-T-P-Credits
CY 405	**Chemical and Statistical Thermodynamics**	**3-0-0: 03**
Prerequisite: NIL		

Course Objectives: The main objective of the course is to provide basic ideas of chemical and statistical thermodynamics and their related aspects. The course is designed for the students to provide the outlines of various laws of equilibrium, non-equilibrium and statistical thermodynamics. The course will be useful to explore the ideas of phase rule in mono and multi-component systems. Further To make conversant the students with the aspects of non-equilibrium thermodynamics and further discussion on various systems of interest.

Course Outcomes: After successful completion of the course, students will be able to:

1. Understand fundamental concepts of chemical and statistical thermodynamics.
2. Understand the ideas of laws of chemical thermodynamics and their related applications in real transformations.
3. Analyze the postulates of non-equilibrium thermodynamics and further discussion of various irreversible processes.
4. Evaluate the partition function for various modes of motions (translational, rotational and vibrational).
5. Apply the key concepts of statistical thermodynamics in case real gases.
6. Design the problems related to different types of ensembles of statistical thermodynamics.

SYLLABUS

Module	Contents	Hours
I	**Equilibrium thermodynamics:** Thermodynamics: Concept of system, exact differentials, Energy and heat changes, reversible processes, heat capacities, relation between C_p and C_v, isothermal and adiabatic process, Joule-Thomson coefficient of ideal and real gases. Thermochemistry: Hess Laws, Heat changes of chemical reactions. Kirchoff's equation and its application, Calculation of heat of reaction from bond energy. Entropy changes in reversible processes; Maxwell's relations, thermodynamic equations of state, variation of entropy with temperature and pressure; Gibbs–Helmholtz equation, criterion of equilibrium, temperature and pressure dependence of equilibrium constant; Vant Hoff equation, Clausius–Clapeyron equation. Partial molar quantities and their determination; Chemical potential and its variation with temperature and pressure; Gibbs–Duhem equation, Concept of fugacity and its determination, ideal solution and non-ideal solutions, activity coefficients and their determination, thermodynamic treatment of solutions; Nernst heat theorem, third law of thermodynamics, residual entropy, free energy and entropy of mixing. Gibbs phase rule: applications to two and three component systems–graphical representation.	14
II	**Non-equilibrium thermodynamics:** Basic concept of non-equilibrium thermodynamics-postulates and methodologies; entropy production in irreversible processes. Linear laws and phenomenological relation: Onsagar reciprocal relation, microscopic reversibility, application to thermoelectric effects: Seebeck, Peltier and	7

	Thompson effect.	
III	**Statistical Thermodynamics**: Concepts of statistical thermodynamics; distribution of molecular states, configuration, ensembles and postulates, canonical ensemble, grand canonical ensemble, micro-canonical ensemble, equivalence of ensembles, thermodynamic Connection, fluctuations, Boltzmann distribution, Bose-Einstein and Fermi-Dirac distribution law; partition functions and interpretation of partition functions. Thermodynamic functions; molar partition functions, evaluation of translational, rotational, vibrational and electronic partition functions; Sackur Tetrode–equation; derivation of thermodynamic properties of ideal gases from partition functions and the ideal gas equation, Real gases: Canonical partition function for interacting particles, intermolecular potential (Lennard-Jones, Hard-sphere and Square-well) and virial coefficients, temperature dependence of the second virial coefficient. Solids: Thermodynamics of solids - Einstein and Debye models. T3 dependence of heat capacity of solids at low temperatures.	15

Essential Readings:

1. P. Atkins and J. D. Paula, "Atkins' Physical Chemistry", Oxford University Press, 10th Edition 2014.
2. B. R. Puri, L. R. Sharma and M. S. Pathania, "Principle of Physical Chemistry", Vishal Publishing Co., 47th Edition 2017.
3. T. Engel, P. Reid, "Thermodynamics, Statistical Thermodynamics and Kinetics", Pearson, 1st Edition 2008.

Supplementary Readings:

1. K. L. Kapoor, "Text Book of Physical Chemistry", Volume 2, Macmillan, 5th Edition 2017.
2. D. A. McQuarrie, "Statistical Mechanics", Viva Books, 1st Edition 2011.