Course Type	Course Code	Name of Course		Т	Р	Credit
DC	NCYC517	Kinetics and Thermodynamics		0	0	3

Course Objective

• Thermodynamics and Kinetics are the foundation of chemistry and it is needed for organic, inorganic and medicinal chemistry. The syllabus was focussed for all branches of thermodynamics, irreversible thermodynamics, statistical thermodynamics apart from classical thermodynamics. The Kinetics part consists of application of basic kinetics concepts to the rate of the reaction.

Learning Outcomes

- Calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential.
- Predict heat capacity of an ideal gas of linear and non-linear molecules from the number of degrees of freedom, rotational and vibrational wavenumbers.
- Calculate transport properties of gases, liquids and solids

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Classical Thermodynamics: Concept of entropy, reversible and irreversible processes, Clausius inequality, Free energies, Criteria of spontaneity. Fundamental equations for open systems, Partial molar quantities and chemical potential, Gibbs-Duhem equation, Real gases and fugacity. Entropy changes in chemical reactions, The Gibbs energy of real gases	12L	Students will be able to review the concepts of classical thermodynamics concepts and be prepared to understand the concepts of non- equilibrium and statistical thermodynamics.
2	Non-equilibrium Thermodynamic: criteria for non-equilibrium states, entropy production, flow, irreversible processes, Electrokinetic phenomena, Diffusion, Electric conduction, Coupled reactions.	8L	Students will have the introduction to the application of the concepts of thermodynamics to non-equilibrium processes and its applications.
3	StatisticalThermodynamics:Concept of ensembles, Canonicalensemble, Boltzmann distribution,Thermodynamic quantities andcanonical partition function. Grandcanonical ensemble, Fermi-Dirac andBose-Einsteindistributions.Molecular partition functions,thermodynamicproperties,Equipartitiontheorem, Chemicalequilibrium.Realgases,intermolecularpotentialandvirial	12L	Students will have the exposure to the concepts of statistical thermodynamics and be able to predict heat capacity of an ideal gas of linear and non-linear molecules from the number of degrees of freedom, rotational and vibrational wavenumbers.

	coefficients. Debye and Einstein theory of heat capacity of		
	solids. Structure and thermal properties of liquids.		
4	Chemical kinetics and applications: Theories of chemical reaction rates, Rate theories based on thermodynamics, Rate theory based on Statistical Mechanics, Conventional Transition State Theory and Applications. Thermodynamics of Adsorption, Catalysis, The role of the surface in catalysis.	10L	Students will have the understanding of conventional and statistical mechanics based rate theories and their applications.
Total		42 L	

Text Books:

1. D. A. McQuarrie, Statistical Mechanics, University Science Books, California 2005.

Reference Books:

- P. Atkins and J. Paula, Physical Chemistry, 8th Edition, Oxford University Press, Oxford 2006.
- 2. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2011.