BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI, PILANI CAMPUS
FIRST SEMESTER 2016-2017
Course Handout Part II Date:26/07/2016

In addition to Part I (General Handout for all courses appended to the time table), this portion gives further specific details regarding the course:

Course No. : CHEM F422
Course Title : Statistical Thermodynamics
Instructor-in-charge : PRASHANT UDAY MANOHAR

Scope and Objective: The course will introduce the students to the principles, methods and applications of statistical thermodynamics. After introducing the concept of ensemble averages, the connection between thermodynamic quantities and the canonical partition function will be established, following which other ensembles and fluctuations will be discussed. Fermi-Dirac, Bose-Einstein, and Boltzmann statistics will then be introduced. The application of Boltzmann statistics to ideal gases and chemical equilibrium will be described, followed by a discussion of ideal quantum gases. The treatment of crystals, and imperfect gases, and an introduction to liquids will form the last section of the course.

Text Book: 'Statistical Mechanics', Donald A McQuarrie, Viva Books Pvt. Ltd., 1st Indian Edn. (2003).

Reference Books:
1. 'Introduction to modern statistical Mechanics', D. Chandler, Oxford University Press, NY (1987).
2. 'Introduction to Statistical Thermodynamics', Terrell L Hill, Addison Wesley (1960).

Course Plan:

Topic	Learning Objectives	Lect	Ref. to text
Review and Introduction	Review of the principles of classical and quantum mechanics, and equilibrium thermodynamics. Introduction to the scope of statistical thermodynamics	3	Ch.1
Canonical Ensemble	Ensemble averages, method of most probable distribution, canonical partition function and the connection to thermodynamics	4	Ch. 2
Fluctuations	Other ensembles, and fluctuations of thermodynamic quantities in different ensembles	3	Ch. 3
Fermi-Dirac, Bose-Einstein, and Boltzmann Statistics	Identical particles, permutation symmetry, F-D and B-E statistics, Boltzmann statistics limit and molecular partition function	4	Ch. 4
Ideal Monatomic Gas	Translational, electronic and nuclear partition functions, thermodynamic functions	2	Ch. 5
Ideal Diatomic Gas	Rigid-Rotator-Harmonic Oscillator approximation, Vibrational and Rotational partition functions, symmetry requirements	3	Ch. 6
Ideal Polyatomic Gas	Normal modes, Rigid-rotators – linear, spherical, symmetric and asymmetric, partition functions	2	Ch. 7
Chemical Equilibrium	Equilibrium constants from partition functions	4	Ch. 9
Quantum Statistics	Ideal Fermi-Dirac gas, electrons in metals, Ideal Bose-Einstein gas, Photon gas	5	Ch. 10 (10.1 to 10.5)
Crystals	Specific heat of crystal – Einstein and Debye theories, lattice dynamics, point defects	4	Ch. 11
Imperfect Gases	Dense gases, virial equation of state, virial coefficients – calculation for model interaction potentials, law of corresponding states	4	Ch. 12
Classical Monatomic Liquids	Distribution functions, radial distribution function and thermodynamic functions, Kirkwood Integral equation, Direct correlation function	3	Ch. 13 (13.1 to 13.5)

Home Assignments: Assignments will be given periodically to supplement the material discussed in class. See Evaluation Scheme below for weightage. These will include problem solving, oral tests, seminars, etc.

Evaluation:

Component	Weightage (%)	Date & Time	Remarks
Midsem	30	*	Closed-book
Assignments	30	periodically	
Comprehensive*	40	*	Closed/Open

*The Comprehensive Examination will have two parts: A closed-book quiz followed by an open book part.

Chamber Consultation Hour: To be announced.

Make-up may be given for genuine case on case-to-case basis. There is no make-up for "Assignments" component.

Notices concerning the course will be displayed on Nalanda and/or Chemistry Dept. Notice Board.

Instructor-in-Charge
CHEM F422