

**BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI-GOA CAMPUS.**  
**INSTRUCTION DIVISION**  
**FIRST SEMESTER 2008-2009**  
**COURSE HANDOUT FOR CHEMICAL THERMODYNAMICS**

**Date: 02/08/2008**

**Course No.** : CHEM C321  
**Course Title** : CHEMICAL THERMODYNAMICS  
**Instructor-in-Charge** : RANJAN DEY

**1. Scope and Objective:** The course is concerned with the energy and the energy changes and is thus related to any kind of energy change occurring in physical, chemical or biological system. It thus belongs to all branches of science and its knowledge equips the scientists to predict the existence of a state or the probability or feasibility of a process to occur at a given temperature and pressure. The course will include a brief introduction to principle and the methods of thermodynamics, which can be basically categorized into three types: equilibrium thermodynamics, non-equilibrium thermodynamics, and statistical thermodynamics.

**2. Text Book(s):**

- (a) Ira N. Levine, *Physical Chemistry*, Tata McGraw-Hill, 2002, 5<sup>th</sup> Ed.
- (b) Donald A. McQuarrie and John D. Simon, *Molecular Thermodynamics*, Viva Book Pvt. Ltd., New Delhi, 2004 (TB2).

**3. Reference Books:**

- (a) K. G. Denbigh, *Principles of Chemical Equilibrium*, Oxford University Press, 1981, 4<sup>th</sup> Ed.
- (b) G. N. Lewis and M. T. Randall (Revised by K. S. Pitzer and L. Brewer), *Thermodynamics*, McGraw-Hill, N.Y., 1961.
- (c) Peter Atkins and Julio de Paula, *Atkins' Physical Chemistry*, Oxford University Press, 2001, 7<sup>th</sup> Ed.
- (d) R.C. Srivastava, Subit K. Saha and Abhay K. Jain, *Thermodynamics*, Prentice Hall of India, 2004, 2<sup>nd</sup> Ed.

#### 4. Course Plan:

Topic	Learning Objectives	Lecture Nos.	Ref. text
Thermodynamics	Thermodynamic systems, concepts of work and heat	1-2	1.2, 1.7, 2.2, 2.3
First Law of Thermodynamics	Law, enthalpy, heat capacities, Joule and Joule-Thompson experiments, state functions	2-4	2.4 to 2.7, 2.10
Second Law of Thermodynamics	Natural & Reversible Processes, Heat Engines, Entropy, Thermodynamic Temperature, Spontaneity & Equilibrium in Isolated Systems	5-8	3.1 to 3.5, 3.7, 4.3
Free Energy and Thermodynamic Relationships	Concepts of Gibbs and Helmholtz energies, Thermodynamic relationships in equilibrium, changes in state functions	9-10	4.4 to 4.6
Third Law of Thermodynamics	Entropy and third law, absolute zero	11	5.7, 5.11
Solutions	Partial molar quantities and their determination, chemical potential, material equilibrium	12-13	9.2 to 9.4, 4.7
Thermodynamics of Ideal Gases	Chemical potential in an ideal gas mixture, ideal-gas reaction equilibrium, temperature dependence of K	14-15	6.1-6.3
Thermodynamics of Real Gases	Compression factors, equations of states, critical data and equations of states, critical states and law of corresponding states	16-17	8.1,8.2,8.4,8.6, 8.7
Reaction Equilibrium	Extent of reaction, condition for equilibrium, standard thermodynamic functions of reaction.	18-20	4.9,5.1-5.3, 5.4 (self study), 5.8, 11.4, 11.5
Phase Changes	Trouton's rule, Clayperon equation	21	7.1, 7.3
Non-ideal Solutions	Activity and activity coefficients, excess functions, Gibbs-Duhem equation	22-23	10.1,10.2,10.3 (p290), 10.4,10.5
Electrolyte Solutions	Ionic activities, ionic interactions, Debye-Huckel Theory	24-25	10.6, 10.8
Electrochemical Systems	Electrochemical systems and their thermodynamics, Galvanic cells Reversible electrodes, thermodynamics of Galvanic cells, liquid junction potential	26-27	14.1 to 14.4 (self study) 14.5-14.9
Surface Chemistry	Adsorption of gases on solids	28	13.5
Statistical Thermodynamics	Micro and thermodynamic states, statistical postulate, ensembles, canonical and molecular partition functions, Boltzmann distribution, perfect gas, thermodynamic properties and equilibrium constant, entropy and third law of thermodynamics	29-33	22.1 to 22.6, 22.8-22.10

Non-equilibrium Thermodynamics-Entropy	Concepts of non-equilibrium thermodynamics, flux-force relation, Onsager reciprocal relation	34-35	14.1-14.4 (TB2)
Electrokinetic Quantities and Onsager's Reciprocal Relations	Application of Onsager's reciprocal relations	36-37	14.5-14.7 (TB2)
Liquid-junction Potential and Transport Numbers	The concept of liquid-junction potential and its relation to transport number	38	14.8 (TB2)
Henderson Equation	Henderson equation and its application to approximation of liquid-junction potential	39	14.9(TB2)
Flux-force Relations and Gradients of Thermodynamic Quantities	The dependence of flux-force relations on gradient of thermodynamic quantities	40	14.10(TB2)
Steady State, Glansdorff-Prigogine (GP) Inequality	Concept of steady state and minimum entropy production, application of GP inequality	41	14.11,14.12 (TB2)

### 5. Evaluation:

EC No.	Component	Duration	Weightage (%)	Date, time, venue	Nature
1	Test I	60 min	25	22/9/08 Mon 8:30AM-9:30PM	CB
2	Test II	60 min	25	5/11/08 Wed 8:30AM-9:30PM	CB
3	Quiz	30 min	10	To be announced in class	OB/CB
3	Comprehensive exam	3 hours	40	05/12/08(AN)	CB

**6. Make-up Policy:** Make up will be granted only in truly deserving cases. Except in cases of extreme emergency, permission must be obtained in advance.

**7. Chamber Consultation Hour:** To be announced

**8. All notices** concerning the course will be displayed on the notice board of the Chemistry Group ( C-Wing).

**9.** Please verify the date, time and venue of the **exams** from the Time Table.

Instructor in Charge  
CHEM C321