

Indian Institute of Science Education and Research, Mohali
Sector 81, S A S Nagar, Manauli PO, Mohali, 140306.
SECOND SEMESTER 2012-2013
Course Handout

Date: 07/01/2013

Course No : **CHM202**
 Course Title : **Energetics and Dynamics of Chemical Reactions**
 Instructor: **Angshuman Roy Choudhury**
 Tutors: **Samrat Ghosh and Angshuman Roychoudhury**

1. Scope and Objective of the Course: The course has been designed to give an overview of classical thermodynamics and their applications in chemical systems and physical phenomenon. The applications of thermodynamics will include chemical equilibrium, phase equilibrium, phase transformations, etc. Basic aspects of chemical kinetics and its applications will also be covered.

2. Text Book: 'The Elements of Physical Chemistry', P.W. Atkins & Julio de Paula, 5th edition, Oxford University Press, Oxford 2006.

3. Reference Books: (1) 'Physical Chemistry', P.W. Atkins & Julio de Paula, 8th edition, Oxford University Press, Oxford 2006, (2) 'Physical Chemistry', Ira Levine, Tata Mcgraw Hill Education Private Limited (2011)

4. Course Plan:

Lect. No	Topics	Learning Objectives
1	Introduction to the course and evaluation components	Introduction to thermodynamics, basic definitions needed to describe thermodynamic systems
2-3		Ideal and real gas laws, van der Waals equation of state, kinetic theory of gases
4-8	Thermodynamics: The Zeroth law The First Law, Internal Energy and Enthalpy	Thermodynamic Systems, State Functions, Thermal Equilibrium and Temperature, Work, Internal Energy and Heat Transfer, Heat Capacity, Equilibrium, Reversibility, Work done for reversible and irreversible processes, calculation of q, w, ΔU and ΔH for ideal and real gases, isothermal and adiabatic transformations.
9-10	Importance of state functions	Mathematical properties, dependence of U on V and T, variation of H with T at constant P, variation of H with P at constant T, relationship between C_p and C_v , Joule-Thomson experiment, liquefaction of a gas.
11-12	Thermochemistry	Application of the first Law to physical and chemical changes, Hess's law, temperature dependence of reaction enthalpies, experimental determination of ΔU and ΔH for chemical reactions, Differential Scanning Calorimetry.
13-15	The Second Law, Entropy, Gibbs Energy, The third law of thermodynamics	Natural and Reversible Processes, Carnot's cycle, Entropy and Second Law, Calculation of Entropy Changes, Clausius inequality, Absolute Entropies, Spontaneity and Equilibrium, ΔS in chemical reactions, dependence of S on V and T, dependence of S on T and P, Gibbs and Helmholtz energy.
16-18	Phase Equilibria of Pure Substances	Intermolecular forces and condensation, Gibbs Energy and Thermodynamics of Phase Transition, Phase boundaries, Gibb's Phase Rule and Phase Diagrams of pure substances.
19-22	Mixtures: Thermodynamic Description, Colligative properties, Phase equilibrium	Partial Molar Properties, Ideal, Ideal-dilute and Real Solutions, elevation of Boiling point and depression of Freezing point, Osmosis pressure, Binary phase diagrams of various liquids, Critical solution temperature, binary eutectic phase diagram
23-24	Chemical Reaction Thermodynamics	Reaction Gibbs Energy, Reaction Quotient, Equilibrium Constant, Coupled Reactions, Response to Conditions.
25-27	Chemical Kinetics	Rate Laws, Order, Rate Constants, Arrhenius Equation, Collision theory, Activated Complex Theory

28-30		Elementary Process, Rate-determining step, Steady-state Approximation, Reactions on Surfaces, Unimolecular Reactions, Reactions in Solution, Catalysis – Homogeneous, Heterogeneous
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5. Evaluation Scheme:

Component	Duration	Full Marks	Date and Time	Remarks
Mid Sem. I	1hr	40		Closed Book
Mid Sem. II	1hr	40		Closed Book
Tutorials		40	Four surprise quizzes during tutorial hour	*
End Sem. Examination	3 hrs.	100		\$

* **Tutorials:** The tutorial hours are designated for quick review of the highlights of the material covered in the lectures, clarification of doubts, and problem solving. Further, set of problems will be assigned periodically. There will likely be 4-6 tutorial test/quiz of 10 marks in each tutorial class, of which best 4 will be taken for final grading. **Students must bring the tutorial problem sheets to the subsequent tutorial session without fail. Students must attend only the tutorial section in which they are registered.**

\$ The Comprehensive Examination will have a closed book quiz portion with and an open or close book descriptive section.

6. **Office Consultation Hours:** To be announced in the class.

7. The tutorial problem sheets, additional exercises, other course related materials will be available on the intranet.

8. **Notices:** Notices, if any, concerning the course will be displayed on the Notice Board of Hostel 5 and Hostel 7 and e-mail will also be sent to all the students.

9. Only **text book, reference book** and **class/tutorial notes** will be allowed in the case of any Open Book exam. **Problem solution manuals, IIT-JEE problem sets and their solutions etc. strictly not allowed in the open book examination.**

10. Ordinary scientific calculators will be allowed. Programmable calculators, calculators with any operating system/extra memory, calculators having graph plotting functions are strictly not allowed in any of the evaluation components.

Instructor
CHM 202