Wednesday, September 15, 2010

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Course: CHMC20H3F, Intermediate Physical Chemistry

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Lectures: Room SW 221, Wednesday 12:00–14:00

Marking Scheme for CHMC20H3F, Fall 2010

Problem Sets	30%
1 Term Test	30%
Final Exam	40%
TOTAL	100%

Required Text: T. Engel and P. Reid, PHYSICAL CHEMISTRY 2nd Edition (Pearson, Toronto, 2010).

Recommended Text: K.J. Laidler, J.H. Meiser, and B.C. Sanctuary, PHYSICAL CHEMISTRY, 4th Edition (Houghton Mifflin, New York, 2003).

In Laidler *et al* for this course the relevant sections are:

Chapter 15, pages 781–830, *Statistical Mechanics*

Chapter 16, section 16.5, pages 874–882, *Statistical Mechanics of Crystals: Theories of Heat Capacities.*

Course Outline

You may already have copy of Engel and Reid from CHMB21H3F.

I suggest that you read all the chapters of your copy (edition) quickly to get an overview.
If your copy is the 1st edition then the chapter numbers and starting pages are as follows: Chapter 30, page 721: Probability; Chapter 31, page 745: The Boltzmann Distribution; Chapter 32, page 767: Ensemble and Molecular Partition Functions; Chapter 33, page 799; Statistical Thermodynamics.

If your copy is the 2nd edition then the chapter numbers are those given below.

29. *Probability Theory* (pages 719–738). This discussion of permutations and combinations is relevant to the treatment of the *Microcanonical Ensemble*.

30. *Boltzmann Distribution* (pages 743–761). This section is related to discussion of the *Canonical Ensemble* where a system interacts with a heat bath at temperature TK.

31. *Ensemble and Molecular Partition Functions* (pages 765–792). This section mentions the *Canonical Ensemble* which I will discuss in detail. Translating, noninteracting molecules, i.e., gas molecules, with internal energy states are a special case of the canonical ensemble where the ensemble partition function is calculated from translational and internal contributions. However, intermolecular forces can easily be treated within the canonical ensemble.

32. *Statistical Thermodynamics* (pages 797–823). The standard thermodynamical functions are can be related to the canonical partition function. and this is done here.

Course Outline in the order in which I will discuss topics: See course the description for CHMC20H3 *Intermediate Physical Chemistry*, page 70, in the UTSC Calendar for 2010–2011.

I will provide typed lecture notes on my lectures in the order in which they are given.

1. *Ensembles:* Microcanonical, Canonical and Grand Canonical

2. *Boltzmann Distribution Law:* Canonical Ensemble, Canonical Partition Function Q

3. *Molecular Partition Functions:* qs of various kinds: translational, rotational, vibrational, electronic

4. *Canonical Partition Function in Calculation of Thermodynamic Functions:* Internal Energy, Enthalpy, Gibbs Energy

5. *Canonical Partition Function in Various Calculations:* Equilibrium Constant, Transition State Theory

6. *Statistical mechanics of Solid State:* Einstein and Debye Heat Capacities

7. *Classical and Quantum Statistics:* Boltzmann, Fermi-Dirac and Bose-Einstein Statistics

8. *Statistical Mechanics of Liquids*