Wednesday, September 13, 2012

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Course: CHMC20H3F, Intermediate Physical Chemistry

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Lectures: Room BV 355, Wednesday 12:00–14:00

Marking Scheme for CHMC20H3F, Fall 2012

Problem Sets	60%
Final Exam	40%
TOTAL	100%

Recommended Texts:
T. Engel and P. Reid, PHYSICAL CHEMISTRY 1^{st} or 2^{nd} Edition (Pearson, Toronto, 2010).
K. J. Laidler, J. H. Meiser, B. C. Sanctuary, PHYSICAL CHEMISTRY 4^{th} Edition (Houghton Mifflin, Reading, Mass, 2003). Now new version is available only electronically.
T. L. Hill, Introduction to Statistical Thermodynamics original version (Addison-Wesley, London, 1960); (Dover Publications, 1987) $19.00US. Look on web using "t l hill dover publications".

There are many good articles on the web.
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.

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 2^{nd} 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. *(Quantum Statistics)*

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

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

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

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

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