Wednesday, September 15, 2010

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Course: CHMC20H3F, Intermediate Physical Chemistry

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 T K.

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