

2011/2012 FIRST SEMESTER LECTURE GUIDE ON SELECTED TOPICS

CHM 331 – PHYSICAL CHEMISTRY III

PART B

MAXWELL – BOLTZMAN'S STATISTICS

1. Introduction and definition of terms:

Configuration and microstates

2. Relating microstates to permutations using probability theory

Identifying predominant configuration

3. Derivation of Stirling's approximation of predominant configuration
4. Derivation of Boltzmann distribution, application of BD to energy levels / spacing and summation of energy over all spacing i.e. partition function

Incorporating degeneracy of energy levels into the partition function

5. Explanation of the physical meaning of the Boltzmann distribution law, relationship between energy, predominant configuration and temperature (outline the principle and derivation of the equation $\beta = 1/k T$)
6. Molecular partition functions

Definition of an ensemble as a collection of identical units of a system

Canonical ensemble as one in which temperature, volume and number of particles in the system are constant.

7. Relate E , W , and probability of E_i to the canonical partition function Q
8. Relate Q to molecular partition function (q) for an ideal gas
9. Evaluating q by molecular energy levels for diatomic molecules possessing four degrees of freedom – rotation, translation, vibration electronic.
10. Symmetry number and partition function
11. Rotational temperature
12. The equipartition theorem – variation of q with temperature

STATISTICAL THERMODYNAMICS

1. Derive an expression for the average and total energy the principles of BD
2. Relate internal energy to the canonical partition function
3. Energy and molecular energetic degrees of freedom: translation, rotation, vibration and electronic
4. Calculation of thermodynamic parameters – entropy, enthalpy and equilibrium constant from partition functions with emphasis on Sackur – Tetrode equation.

INTRODUCTORY QUANTUM CHEMISTRY

1. Why study Q M ? meaning of QM
2. Origin of QM: theory and experiments.

Blackbody radiation and the photoelectric effect.