

CBE 310 Molecular Concepts and Applications

Temperature and Heat Capacity Ensembles and Partition Functions

10 27 2014

Topics for today:

- 1) Quick Review of Statistical Mechanics
- 2) Definitions and relations of Temperature and Heat Capacity
- 3) Aside: Ensembles, a different formulation of statistical mechanics
- 4) Introduction to Chemical Equilibria
Handout on the topics for today posted

Wednesday	10/29	: Quiz #3
Friday	10/31	: Equilibrium Constants Handout / Reading for Monday
Monday	11/03	: Equations of State
Wednesday:	11/05	: Structure of Liquids
Friday	11/07	: PLI Day
Monday	11/10	: Kinetic Theory of Gasses
Wednesday	11/12	: Kinetic Theory of Gasses
Friday	11/14	: Electrolytes and Diffusion
Monday	11/17	: Statistical Mechanics Overview
Wednesday	11/19	: Quiz 4
Friday	11/21	: Protein Folding and Statistical Thermodynamics
FALL BREAK	11-24 to 11-28	

Statistical Mechanics provides the bridging connection between microscopic world governed by the laws of quantum mechanics and the macroscopically observable world that is described by thermodynamics.

The macroscopically observable quantities such as temperature, pressure, entropy, free energy, heat capacity, chemical potential, viscosity, spectra, reaction rates, etc. can be derived and /or explained as the **average properties** of large collections of individual molecules with particular quantum mechanically allowed behaviors

Statistical
properties of
large assemblies

$$\frac{n_i}{N} = \frac{1}{\sum_i e^{-\beta \epsilon_i}} e^{-\beta \epsilon_i}$$

$\beta = \frac{1}{kT}$

Partition Functions:
Relation to Internal
Energy and Entropy and
thus all of
thermodynamics

The Boltzmann distribution describes the probability that particles will have a given energy as a function of temperature

$$q = \sum_{\text{all states}} g_i e^{-\beta \epsilon_i}$$

g_i is the degeneracy of a state

q is the **molecular partition function** that describes the number of thermally accessible states of the system. It can be thought of as a sort of “thermal wavefunction”, it contains all of the information necessary to calculate the thermodynamic properties of a system.